5:00 – 6:30 PM, SUNDAY TUTORIAL LECTURES Ballroom B

5:00 pm The Art of Communication in the Sciences



Willard W. Harrison, University of Florida

5:45 pm **Ion Mobility in Mass Spectrometry**



David E. Clemmer, Indiana University

6:45 – 7:45 PM, SUNDAY CONFERENCE OPENING AND PLENARY LECTURE Exhibit Hall C

6:45 pm Welcome to the 57th ASMS Conference on Mass Spectrometry

Gary L. Glish, President, ASMS

7:00 pm Biofuels and Global Climate Change



Jerald L. Schnoor, University of Iowa

7:45 – 9:30 pm WELCOME RECEPTION IN THE EXHIBIT HALL Exhibit Hall AB

8:30 – 10:30 AM, MONDAY MORNING MASS SPECTROMETRY OF LIPIDS Ballroom A

MOA am 8:30 New Insights into the Human Lens through
Multi-Faceted Lipid Mass Spectrometry; Jane
M. Deeley¹; Jessica R. Nealon¹; Roger J.W.
Truscott²; Stephen J. Blanksby¹; Todd W.

Mitchell¹; ¹University of Wollongong,
Wollongong, Australia; ²University of Sydney,
Sydney, Australia

MOA am 8:50 Automated Lipid Identification and Quantitation by Multidimensional Mass Spectrometry-Based Shotgun Lipidomics; Kui Yang; Hua Cheng; Richard Gross; Xianlin Han; Washington University, St. Louis, MO

MOA am 9:10 Methodology for the Rapid Determination of Lipids Employing Chip-Based Nano-ESI FT-ICR MS, Accurate Mass, and Infrared Heating; Larry Lerno; Carlito Lebrilla; University of California, Davis, CA

MOA am 9:30

Identification of a Class of Endogenous
Sulfated Glycosphingolipids in NSC11
Glioblastoma Cancer Stem Cells; Huan He^{1,2};
Mark R. Emmett²; Carol Nilsson³; Alan G.
Marshall²; Howard Colman⁴; Charles A. Conrad⁴;

Iflorida State University, Tallahassee, FL; ²Nat'l
High Magnetic Field Lab, Tallahassee, FL;

³Pfizer, Inc., San Diego, CA; ⁴M.D. Anderson
Cancer Center, Houston, TX

MOA am 9:50 The Comparative Lipidomics of VSV, SFV and their Host Plasma Membrane by Quantitative Shotgun Mass Spectrometry; Julio L Sampaio¹; Lucie Kalvodova²; Christer Ejsing¹; Kai Simons¹; Andrej Shevchenko¹; ¹MPI-CBG, Dresden, Germany; ²Infectious Disease Research Institute, Seattle, Washington

MOA am 10:10 From Single Cells to Whole Body Sections:
Multiscale Imaging of Phospholipids by
MALDI MS; Pierre Chaurand; Peggi Angel;
Richard M. Caprioli; Vanderbilt University,
Nashville, TN

8:30 – 10:30 AM, MONDAY MORNING CHROMATOGRAPHY-MASS SPECTROMETRY APPROACHES TO INCREASE THROUGHPUT IN DISCOVERY PK ASSAYS

Ballroom B

MOB am 8:30 **High Throughput LC-MS in ADME/TOX: Making the Impossible Possible**; <u>Li Di</u>; Edward Kerns; Susan Petusky; Susan Li; Zhen Lin; Guy Carter: Wyeth Research. Monmouth Jct.. NJ

MOB am 8:50 Enhancing the Throughput of Discovery PK
Using High Resolution Ultrafiltration LC-MS;
Richard B. Van Breemen; University of Illinois,
Chicago, IL

MOB am 9:10 Microflow UPLC/MS as a Method to Improve Discovery PK Throughput; Heather E Skor; David C Gale; Sadayappan V Rahavendran; Pfizer Global Research & Development, La Jolla,

MOB am 9:30 Comparison of HPLC-MS/MS and UPLC-MS/MS Performances for Quantification of a Clinical Candidate and its Metabolites in Plasma Utilizing Chemometric Approach;

Margret Thorsteinsdottir^{1,2}; Gisli Bragason²;

Baldur Bragi Sigurdsson²; Olafur Þ Magnusson²;

**Inniversity of Iceland, Reykjavik, Iceland;

2deCODE genetics, Reykjavik, Iceland

Page S8			5/" ASMS Conference on Mass Spectrometry
MOB am 9:50 MOB am 10:10	Fast Determination of Metabolic Soft Spots by New LC/MS Technologies: An Effective Approach to Improving PK Proprieties; Mingshe Zhu; Qian Ruan; Ming Yao; Bristol- Myers Squibb, Princeton, NJ A Novel and Integrated Platform for Fully Automated High-Throughput LCMSMS Analysis of in vitro ADME Samples; Andreas H. Luippold; Thomas Arnhold; Wolfgang Joerg; Klaus Klinder; Kurt Schumacher; Boehringer Ingelheim Pharma GmbH & Co KG, Biberach An Der Riss, Germany	MOD am 9:10	¹ University of Cambridge, Cambridge, United UK; ² Waters Corporation, Manchester, UK Improving the Accuracy of Experimental and Theoretical Cross-Section Measurements in Travelling Wave Ion Mobility Spectrometry-Mass Spectrometry; Tom W. Knapman ¹ ; Joshua T. Berryman ¹ ; Victoria L Morton ¹ ; Iain D G Campuzano ² ; Sarah A. Harris ¹ ; Peter G Stockley ¹ ; Alison E. Ashcroft ¹ ; ¹ Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds UK; ² Waters Corporation, Manchester, UK
9.20	- 10:30 AM, MONDAY MORNING	MOD am 9:30	Deriving a Theoretical Mass Scale from Ion
	IZING PROTEIN-PROTEIN INTERACTIONS	11102 4111 7.50	Mobility Measurements; Stephen Valentine;
CHARACTER	Room 201		David E. Clemmer; <i>Indiana University</i> ,
MOC 9-20			Bloomington, IN
MOC am 8:30	Investigation of Intact Protein Complexes and	MOD am 9:50	Separation of Ion Electronic States by
	Protein-Protein Interactions by Native Ion	WOD am 7.50	Cryogenic Ion Mobility-Mass Spectrometry;
	Mobility and Tandem Mass Spectrometry;		Jody May; David H. Russell; Texas A&M
	Esther Van Duijn; Arjan Barendregt; Charlotte		University, College Station, TX
	Uetrecht; Kristina Lorenzen; Rebecca Rose; Glen	MOD om 10:10	
	Shoemaker; Albert J.R. Heck; Utrecht University,	MOD am 10:10	Integrated 'Omics' on the Basis of Structural
	Utrecht, Netherlands		Separations by Ion Mobility-Mass
MOC am 8:50	Micelles Protect ATP Synthases from Solution		Spectrometry; <u>Larissa S. Fenn</u> ; Michal Kliman;
	to Gas Phase and Reveal Novel Protein		Thomas J. Kerr; Randi Gant; Ablatt Mahsut;
	Interactions in Membrane Embedded		Sophie Zhao; John A. McLean; Vanderbilt
	Subunits; Carol Robinson; Min Zhou; Dijana		University, Nashville, TN
	Matak Vinkovic; Nina Morgner; Shoshanna		– 10:30 AM, MONDAY MORNING
	Isaacson; Neslon Barrera; University of	QUANT	ITATIVE BOTTOM UP PROTEOMICS
	Cambridge, Cambridge, UK		Exhibit Hall C
MOC am 9:10	Transient Protein Interactions and Ligand	MOE am 8:30	Designing, Executing, and Analyzing
	Exchange between Transporters and		Quantitative Bottom Up Proteomics Studies for
	Receptors: MS Study of Retinoic Acid Delivery		Biological Discovery; Michael Washburn;
	to RAR by CRABP; Virginie Sjoelund; Igor A.		Stowers Institute for Medical Research, Kansas
	Kaltashov; University of Massachusetts, Amherst,		City, MO
	MA	MOE am 8:50	Quantitative MS Proteomics with ¹⁴ N/ ¹⁵ N
MOC am 9:30	Comprehensive Structural Mass Spectrometry	MOE am 8:50	Metabolic Labelling: Precision, Accuracy and
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5/ ASMS Conf	erence on Mass Spectrometry
	David C. Muddiman; North Carolina State University, Raleigh, NC
FUNDAME	- 10:30 AM, MONDAY MORNING NTALS AND NOVEL APPLICATIONS OF ION/MOLECULE REACTIONS Room 103
MOF am 8:30	Gas Phase Reactions of Carbanions with N and
Wor um 0.30	O Atoms ; Zhibo Yang; Brian Eichelberger; Oscar Martinez Jr.; Momir Stepanovic; Theodore P. Snow; Veronica M. Bierbaum; <i>University of</i>
MOF am 8:50	Colorado, Boulder, CO Direct Observation of the Reactions of the Phenyl Radical with Dioxygen Using Distonic Ions; Benjamin B. Kirk; David G Harman;
MOF am 9:10	Stephen J Blanksby; University of Wollongong, Wollongong, Australia Ion Molecule Ghostbusters: Tracking Ephemeral Radical Migration in Peptides and
	Proteins; Benjamin Moore ¹ ; Tony Ly ¹ ; Stephen J. Blanksby ² ; <u>Ryan R. Julian</u> ¹ ; ¹ University of California, Riverside, Riverside, CA; ² University of Wollongong, Wollongong, Nsw, Australia
MOF am 9:30	Ion/Molecule Reactions at Atmospheric Pressure with ESSI-MS: Fundamentals and Applications; <u>David Touboul</u> ^{1,2} ; Matthias Jecklin ² ; Renato Zenobi ² ; ¹ CNRS-ICSN, Gif-sur-
MOF am 9:50	yvette, France; ² ETH Zürich, Zürich, Switzerland Ionization Mechanisms Related to Negative Ion APPI, APCI, and DART; Charles N. McEwen ¹ ; Barbara S. Larsen ² ; ¹ Univ. of the Sciences in PA,
MOF am 10:10	Philadelphia, PA; ² The DuPont Company, Wilmington, DE Data Dependent Neutral Gain MS3: Toward Automated Functional Group Identification in Drug Metabolites via LC-MS, Ion-Molecule
	Reactions and CAD; Steven Habicht; Nelson Vinueza; Hilkka Kenttamaa; Purdue University, West Lafayette, IN
	– 10:30 AM, MONDAY MORNING IN ELEMENTAL MASS SPECTROMETRY
	Room 113
MOG am 08:30	Bio-Imaging of Metals in the Brain by Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) to Study
MOG am 8:50	Neurodegenerative Diseases; Johanna Sabine Becker; Forschungszentrum Juelich, Juelich, Germany Cytotoxicity of Arsenic Containing Chemical
	Warfare Agent Degradation Products with Metallomic Approaches for Metabolite Analysis; Karolin K. Kroening ¹ ; Renee N. Easter ¹ ; Morwena J.V. Solivio ¹ ; Alvaro Puga ² ; Joseph A. Caruso ¹ ; <i>Dept. of Chemistry, UC, Cincinnati, OH</i> ; <i>Dept. of Environmental Health</i> ,
MOG am 9:10	UC, Cincinnati, OH Speciation Analysis of Gadolinium Chelates in Hospital Effluents and Wastewater Treatment Plant Sewage by a Novel HILIC/ICP-MS Method; Jens Künnemeyer; Lydia Terborg; Björn Meermann; Christine Brauckmann; <u>Uwe Karst;</u>
MOG am 9:30	University of Münster, Münster, Germany Characterization of Selenium Metabolites in Se-enriched Kale via Ion-Pairing Reversed Phase Chromatography with ICPMS and ESI

Phase Chromatography with ICPMS and ESI-

IT-MS Detection; <u>Qilin Chan</u>; Scott E. Afton; Joseph A. Caruso; *Department of Chemistry*,

University of Cincinnati, Cincinnati, OH

MOG am 9:50

Elucidating the Role of Metals in Amyotrophic Lateral Sclerosis Using Inline Liquid Chromatography- Inductively Coupled Plasma- Mass Spectrometry; Lelie Herman¹; Liba Amir²; Pik Chan³; Joan Valentine¹; Julian Whitelegge³; ¹University of California, Los Angeles, Los Angeles, CA; ²Agilent, Wilmington, DE; ³University of California LA, Los Angeles, CA

MOG am 10:10

Separation and Quantification of Antisense Oligonucleotides by Hydrophilic Interaction Liquid Chromatography Coupled to ICP-MS.; Renee N. Easter; Karolin K. Kroening; Patrick A. Limbach; Joseph A. Caruso; University of

10:30 AM – 2:30 PM, MONDAY POSTER SESSION Exhibit Hall AB

Cincinnati, Cincinnati, OH

2:30 – 4:30 PM, MONDAY AFTERNOON MS AND ACCELERATOR MS FOR HUMAN MICRODOSING AND METABOLISM STUDIES Ballroom A

MOA pm 2:30 A Review of the State-of-the Art of human Microdosing and Nanotracer Studies - as an Introduction to the Session; Graeme Young; GlaxoSmithKline

MOA pm 2:50 Absolute Quantitation without Internal

Standards: Accelerator Mass Spectrometry and Microtracers for Pharmacokinetics and Metabolite Discovery; Pete Lohstroh; Brad Keck; Le Vuong; John Vogel; Stephen Dueker; Vitalea Science, Davis, CA

MOA pm 3:10 Quantification and Identification of
Metabolites at Microdosing Levels; Carmai
Seto¹; Takeo Sakuma¹; Jinsong Ni²; Fred
Ouyang²; Devin Welty²; Van Dinh²; Gabriella
Szekely-klepser²; Andrew Acheampong²; ¹MDS
Analytical Technologies, Concord, Canada;
²Allergan Inc., Irvine, CA

MOA pm 3:30 Single Instrument AMS and IRMS for

Microdose/Microtrace Mass Balance Studies;

Giacomo Jason¹; Tim Schulz-König²; Stephen

Dueker¹; Brad Keck¹; Hans-Arno Synal²; John

Vogel¹; Vitalea Science, Davis, CA; ²ETH

Zurich, Zurich, Switzerland

MOA pm 3:50 **Early Investigation of Human Metabolism in Drug Development**; <u>David S. Wagner</u>; Amanda
Culp; John Ulrich; Andrea Sefler; Steve
Castellino; *GlaxoSmithKline, Rtp, NC*

MOA pm 4:10 Comprehensive Analysis of (Phosphorylated)
Nucleoside Reverse Transcriptase Inhibitors
and Endogenous Deoxynucleotides in Plasma
and PBMCs Using (Ion-Pair) LC-MS/MS; Leon
Coulier; Henk Gerritsen; Lars Brull; TNO Quality
of Life, Zeist, Netherlands

2:30 – 4:30 PM, MONDAY AFTERNOON MASS SPECTROMETRY AND CLINICAL APPLICATIONS Ballroom B

MOB pm 2:30 Dermcidin Identification from Exhaled Air for Lung Cancer Diagnosis; Wei-chao Chang¹; Ming-Shyan Huang²; Chih-Jen Yang²; Wen-Yu Wang²; Tsung-Ching Lai¹; Michael Hsiao¹; Chung-Hsuan Chen¹; ¹The Genomics Research Center, Academia Sinica., Taipei, Taiwan;

using a Pulsed Valve and Increased Drive

Frequency; Bruce Collings; Matthew A.

²Kaohsiung Medical University Hospital, Gary Asmussen; Tatiana Gladysheva; James Kaohsiung, Taiwan Lillie; Aharon Cohen; Bing Wang; Genzyme MOB pm 2:50 **Large-Scale Proteomic Study of Chronic** Corporation, Waltham, MA MOC pm 3:30 Kidney Allograft Rejection from Tissue **Probing the Gas-Phase Dissociation Behavior** Biopsies; Aleksey Nakorchevsky¹; Johannes of Model Homodimeric Protein Complexes Hewel²; Daniel Salomon¹; John Yates¹; ¹The with Divergent Interfacial Structures; Eric D. Scripps Research Institute, La Jolla, CA; Dodds; Anne E. Blackwell; Christopher M. Jones; ²University of Toronto, Toronto, ON Matthew H. J. Cordes; Vicki H. Wysocki; MOB pm 3:10 **Targeted MRM Expression Profiling of 45** University of Arizona, Tucson, AZ Proteins in a Cohort of 60 Cardiovascular MOC pm 3:50 Sequence analysis of Intact Disulfide-Rich Disease Plasma Samples; Michael A. Kuzyk¹; Mini-Proteins Using a Combined Chemical Darryl B. Hardie¹; Gabriela Cohen-Freue²; Derivatization and ETD Strategy; Beatrix <u>Ueberheide</u>¹; David Fenyo¹; Paul F Alewood²; Dominik Domanski¹; Juncong Yang¹; John S. Hill²; Angela M. Jackson¹; Christoph H. Brian Chait¹; ¹The Rockefeller University, New Borchers [; ¹UVic-Genome BC Proteomics Centre, York, NY; ²The University of Queensland, St Victoria, Canada; ²James Hogg iCAPTURE Lucia, Australia MOC pm 4:00 Top-Down Proteomics with a 14.5 T FT-ICR Centre, Vancouver, Canada MOB pm 3:30 Sensitive Quantification of Circulating Vitamin Mass Spectrometer: Secondary Ion Collection D Metabolites in Multiple Sclerosis Patients in an External Octopole Ion Trap; Jeremiah D. <u>Tipton</u>¹; John F. Kellie^{2,3}; Paul M. Thomas^{2,3} Using Selective SPE coupled to Capillary-LC and Isotope-Dilution MS; Xiaotao Duan^{1,2}; Eunjin Bang¹; Hao Wang^{1,2}; Bianca Weinstock-Dorothy R. Ahlf^{2,3}; Chris L. Hendrickson^{1,4}; Neil L. Kelleher^{2,3}; Alan G. Marshall^{1,4}; ¹National Guttman¹; Murali Ramanathan¹; Jun Qu^{1,2}; High Magnetic Field Laboratory, Tallahassee, ¹University at Buffalo, Amherst, NY; ²CoE FL; ²Department of Chemistry, UI, Urbana-Champaign, IL; ³Institute for Genomic Biology, Bioinformatics & Life Sci, Buffalo, NY UI, Urbana-Champaign, IL; ⁴Department of MOB pm 3:50 Ultra High-Throughput Quantitative LC-MS/MS in a Clinical Diagnostics Laboratory -Chemistry, FSU, Tallahassee, FL Breaking the 2000 Samples/System/Day 2:30 - 4:30 PM, MONDAY AFTERNOON Barrier; Russell Grant; Brian Rappold; Patricia DEVELOPMENTS IN ION TRAPPING Holland; LabCorp, Burlington, NC INSTRUMENTATION MOB pm 4:10 Quantitative Human Plasma Protein Room 204 Biomarker Verification by Multiple Reaction A New Tool for High-speed Proteomics: MOD pm 2:30 Monitoring: A Multi-site Study of Precision Orbitrap Mass Analyzer Interfaced to a Dual and Reproducibility; Terri Addona¹; Susan E. **Linear Trap**; Eugen Damoc¹; Eduard Denisov¹; Abbatiello¹; Birgit Schilling²; Steven J. Skates³; D. R. Mani¹; David M Bunk⁴; Clifford H. Jens Griep-raming¹; Hartmut Kuipers¹; Oliver Lange¹; Alexander Makarov¹; Philip M Remes²; Spiegelman⁵; Lisa J. Zimmerman⁶; Amy-Joan L. Jae C. Schwartz²; Dennis Taylor²; Thomas Ham⁶; Hasmik Keshishian¹; Steven C. Hall⁷; Moehring¹; Vlad Zabrouskov²; ¹Thermo Fisher Steven A. Carr¹; CPTAC Network⁸; ¹Broad Scientific (Bremen) GmbH, Bremen, Germany; Institute, Cambridge, MA; ²Buck Institute for Age ²Thermo Fisher Scientific (San Jose), San Jose, Research, Novato, CA; ³Massachusetts General Hospital, Boston, MA; ⁴NIST, Gaithersburg, MD; MOD pm 2:50 **Optimized Cell Geometry for Fourier** ⁵Texas A&M University, College Station, TX; Transform Ion Cyclotron Resonance Mass ⁶Vanderbilt University, Nashville, TN; ⁷UCSF, Spectrometry; Christopher L. Hendrickson¹ San Francisco, CA; ⁸National Cancer Institute, Steven C. Beu²; Greg T. Blakney¹; Nathan Bethesda, MD Kaiser¹; Daniel G. McIntosh¹; John P. Quinn¹; Alan G. Marshall^{1,3}; ¹National High Magnetic 2:30 - 4:30 PM, MONDAY AFTERNOON TANDEM MS OF WHOLE PROTEINS AND PROTEIN Field Laboratory, Tallahassee, FL; ²S C Beu **COMPLEXES** Consulting, Austin, TX; ³Florida State University, Room 201 Tallahassee, FL MOC pm 2:30 Revealing the Sites of Ligand and Protein MOD pm 3:10 Femtosecond Laser-Induced Ionization/ Binding in Protein Complexes by Top-Down Dissociation (fs-LID) of Protonated Mass Spectrometry; Sheng Yin; Joseph A. Loo; Biomolecules; Christine L. Kalcic; Scott A. UCLA, Los Angeles, CA Smith; Yuanxing Chen; Nelson Winkler; Gavin E. MOC pm 2:50 A High Throughput Format for Top Down Reid; A. Daniel Jones; Marcos Dantus; Michigan **Proteomics Using GELFrEE Coupled to** State University, East Lansing, MI Nanocapillary-LTQ FT ICR MS at >12 Tesla; MOD pm 3:30 Miniature Monolithic Rectilinear Ion Traps <u>Ji Eun Lee¹</u>; John F. Kellie¹; John C. Tran¹; and Arrays by Stereo-lithography on Printed Adaikkalam Vellaichamy¹; Dorothy Ahlf¹; Circuit Board (SLA-on-PCB); Jeff Maas¹; Scott Smith²; Zheng Ouyang¹; R. Graham Cooks¹; William Chappell¹; ¹Purdue University, W. Jeremiah D. Tipton²; Alan G. Marshall^{2,3}; Neil L. Kelleher¹; ¹University of Illinois, Urbana, IL; ²National High Magnetic Field Laboratory, Lafayette, IN; ²Michigan State University, East Tallahassee, FL; ³Florida State University, Lansing, MI Tallahassee, FL MOD pm 3:50 Improvements to MS3 Fragmentation MOC pm 3:10 **High Throughput Quantitative Screening** Efficiency in a Low Pressure Linear Ion Trap

Measuring Intact Proteins by a Novel Rapid

Mass Spectrometric Approach; Kim Alving;

0, 1101110 0011	terence on wass spectrometry		Page S11
	Romaschin; MDS Analytical Technologies,	MOF pm 2:50	Deprotonation Site Determined by IR
	Concord, Canada	•	Spectroscopy; Jos Oomens; Jeffrey D. Steill;
MOD pm 4:10	Electron Ionization Dissociation in a Radio		FOM Rijnhuizen, Nieuwegein, Netherlands
P	Frequency Linear Ion Trap; Atim A. Enyenihi;	MOF pm 3:10	Photofragmentation Spectroscopy of
	Takashi Baba; Gary L. Glish; <i>University of North</i>	mor pms.ro	Protonated Peptides Assisted by Pulsed CO ₂
	Carolina, Chapel Hill, NC		Laser; Oleg V. Boyarkin; Monia Guidi; Natalia S.
2.20	_		
	- 4:30 PM, MONDAY AFTERNOON		Nagornova; Thomas R. Rizzo; <i>LCPM</i> , <i>EPFL</i> ,
BIO	MARKER DISCOVERY – PROTEINS	MOE 2.20	Lausanne, Switzerland
	Exhibit Hall C	MOF pm 3:30	Infra Red Spectroscopy of Fragment Ions of
MOE pm 2:30	Protein Biomarkers: Translating Discoveries		Protonated Peptides; Benjamin Bythell ² ; Undine
-	into Tools; Douglas M. Sheeley; National Center		Erlekam ³ ; Michael J. Van Stipdonk ¹ ; Bela Paizs ² ;
	for Research Resources, Bethesda, MD		Philippe Maitre ³ ; ¹ Wichita State University,
MOE pm 2:50	An Integrative Biology Approach for Plasma		Wichita, KS; ² DKFZ, Heidelberg, Heidelberg,
· r	Biomarker Discovery in Idiopathic Pneumonia		Germany; ³ Laboratoire de Chimie Physiq, Orsay,
	Syndrome; Daniela M Schlatzer ¹ ; Mark R.		France
	Chance ¹ ; Rob M. Ewing ¹ ; Sergei Ilchenko ¹ ;	MOF pm 3:50	Energy Dependent VUV Photodetachment
	Gaurav S.J.B Rana ¹ ; Kenneth R. Cooke ^{1,2} ; ¹ Case	•	Spectroscopy of Polyanions in the Gas Phase
	Western Reserve University, Cleveland, OH;		Probed by Synchrotron Radiation; Alexandre
			Giuliani ^{1,2} ; Debora Scuderi ³ ; Joel Lemaire ³ ;
MOE 2.10	² University Hospitals, Cleveland, OH		Christophe Dehon ³ ; Roland Thissen ⁴ ; Denis
MOE pm 3:10	Protein Cartography of the Tissue		Duflot ⁵ ; Laurent Nahon ¹ ; Philippe Maitre ³ ;
	Microenvironment in Tumor Progression;		Synchrotron Soleil, Gif-sur-yvette, France;
	Thomas P. Conrads ^{1,3} ; Brian L Hood ^{1,3} ; Melanie		² Cepia INRA, Nantes, France; ³ Laboratoire de
	Flint ^{1,3} ; Jaqueline M. Jones-Laugner ^{1,3} ; Arash		Chimie Physique, Orsay, FRANCE; ⁴ Laboratoire
	Radfar ^{2,3} ; Rajiv Dhir ^{2,3} ; ¹ Department of		de Planétologie de Grenoble, Grenoble, France;
	Pharmacology & Chemical Biology, Pittsburgh,		⁵ Laboratoire de Physique des Lasers, Atomes et
	PA; ² Department of Pathology, Pittsburgh, PA;		Mo, Villeneuve d'Ascq, France
	³ University of Pittsburgh Cancer Institute,	MOE nm 4:10	
	Pittsburgh, PA	MOF pm 4:10	Electronic Action Spectroscopy of the GFP
MOE pm 3:30	Studying Biological Variation of Plasma		Model Chromophore in a Quadrupole Ion
	Protein Levels in a Twin Sample Set Using		Trap: Electron Photodetachment vs.
	Targeted Multiplexed MRM Protein		Photodissociation; Matthew W. Forbes; Charles
	Expression Profiling; Christie L Hunter ¹ ; Sean L.		S. Yeung; Chloe Yang; Vy M. Dong; Rebecca A.
	Seymour ¹ ; Veronica Saenz-vash ² ; Marjorie		Jockusch; <i>University of Toronto, Toronto, ON,</i>
	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ;		Canada
	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad		Canada - 4:30 PM, MONDAY AFTERNOON
	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad		Canada – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL
	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad Institute, Cambridge, MA; ⁴ Plasma Proteome		Canada 1 – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY
	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad Institute, Cambridge, MA; ⁴ Plasma Proteome Institute, Washington, DC	MASS SI	Canada 1 – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY Room 113
MOE pm 3:50	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad Institute, Cambridge, MA; ⁴ Plasma Proteome Institute, Washington, DC A Case Study for Shifting the Biomarker		Canada 1 – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY Room 113 The Use of Mass Spectrometry to Support Risk
MOE pm 3:50	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad Institute, Cambridge, MA; ⁴ Plasma Proteome Institute, Washington, DC A Case Study for Shifting the Biomarker Discovery Paradigm: Predicting Response to	MASS SI	Canada 1 – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY Room 113 The Use of Mass Spectrometry to Support Risk Assessment; Michael G. Bartlett; Yongzhen Liu;
MOE pm 3:50	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad Institute, Cambridge, MA; ⁴ Plasma Proteome Institute, Washington, DC A Case Study for Shifting the Biomarker	MASS SI	Canada 1 – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY Room 113 The Use of Mass Spectrometry to Support Risk
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MOE pm 3:50 MOE pm 4:10	Minkoff ¹ ; Steven A. Carr ³ ; Leigh Anderson ⁴ ; ¹ Applied Biosystems, Foster City, CA; ² Broad Institute of MIT and H, Cambridge, MA; ³ Broad Institute, Cambridge, MA; ⁴ Plasma Proteome Institute, Washington, DC A Case Study for Shifting the Biomarker Discovery Paradigm: Predicting Response to Therapy in Hepatitis C Patients Using Unbiased Proteomics; J. Will Thompson ¹ ; Joseph Lucas ² ; Laura G. Dubois ¹ ; Keyur Patel ³ ; Arthur Moseley ¹ ; Diane Uzarski ³ ; Hans Tillman ³ ; Robert Califf ³ ; Geoff Ginsburg ² ; Jeanette Mccarthy ² ; John McHutchison ³ ; ¹ Duke University School of Medicine, Durham, NC; ² Duke Institute for Genome Sciences & Policy, Durham, NC;	MASS SI MOG pm 2:30	Canada 1 – 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY Room 113 The Use of Mass Spectrometry to Support Risk Assessment; Michael G. Bartlett; Yongzhen Liu; Catherine White; Srinivasa Muralidhara; James Bruckner; University of Georgia, Athens, GA Mass Spectrometry Studies of Arsenic Metabolism and Toxicity; Meiling Lu²; Zhongwen Wang³; Anthony McKnight-Whitford¹; Jie Liu¹; Huiming Yan¹; Xiufen Lu¹; Chungang Yuan⁴; Hailin Wang²; X. Chris Le¹; ¹University of Alberta, Edmonton, Canada; ²Res. Centre for
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MOE pm 4:10	Minkoff¹; Steven A. Carr³; Leigh Anderson⁴; ¹Applied Biosystems, Foster City, CA; ²Broad Institute of MIT and H, Cambridge, MA; ³Broad Institute, Cambridge, MA; ⁴Plasma Proteome Institute, Washington, DC A Case Study for Shifting the Biomarker Discovery Paradigm: Predicting Response to Therapy in Hepatitis C Patients Using Unbiased Proteomics; J. Will Thompson¹; Joseph Lucas²; Laura G. Dubois¹; Keyur Patel³; Arthur Moseley¹; Diane Uzarski³; Hans Tillman³; Robert Califf³; Geoff Ginsburg²; Jeanette Mccarthy²; John McHutchison³; ¹Duke University School of Medicine, Durham, NC; ²Duke Institute for Genome Sciences & Policy, Durham, NC; ³Duke Clinical Research Institute, Durham, NC A Robust Mass Spectrometry-Based Pipeline for Biomarker Discovery and Verification; Chenwei Lin¹; Liming Hou¹; Mary Trute¹; Jeffrey R. Whiteaker¹; Alexei Krasnoselsky¹; Regine M. Schoenherr¹; Li-Chia Feng¹; Karen S. Spratt¹; Sharon Pitteri¹; Ted Holzman¹; Ted Whitmore²; Philip Gafken¹; Lisa A. Jones¹; Jason M. Hogan¹; Samir Hanash¹; Christopher J. Kemp¹; Dan Martin²; Martin McIntosh¹; Peter Nelson¹; Amanda Paulovich¹; ¹Fred Hutchinson Cancer Research Center, Seattle, WA; ²Institute For System Biology, Seattle, WA - 4:30 PM, MONDAY AFTERNOON ION SPECTROSCOPY Room 103	MASS SI MOG pm 2:30 MOG pm 2:50 MOG pm 3:10 MOG pm 3:30	Canada 1 — 4:30 PM, MONDAY AFTERNOON PECTROMETRY IN ENVIRONMENTAL TOXICOLOGY Room 113 The Use of Mass Spectrometry to Support Risk Assessment; Michael G. Bartlett; Yongzhen Liu; Catherine White; Srinivasa Muralidhara; James Bruckner; University of Georgia, Athens, GA Mass Spectrometry Studies of Arsenic Metabolism and Toxicity; Meiling Lu²; Zhongwen Wang³; Anthony McKnight-Whitford¹; Jie Liu¹; Huiming Yan¹; Xiufen Lu¹; Chungang Yuan⁴; Hailin Wang²; X. Chris Le¹; ¹University of Alberta, Edmonton, Canada; ²Res. Centre for EcoEnviron, Beijing, CHINA; ³Health Canada, Ottawa, Canada; ⁴North China Electric Power Univesity, Baoding, China SILAC and Mass-Spectrometry for the Assessment of Effects of Arsenite on the Global Protein Expression in the Human HL-60 Cells; Lei Xiong; Yinsheng Wang; University of California, Riverside, CA Monitoring DNA Damaging Exposure Thresholds for a Foodborne Carcinogen Using LC-MS/MS and DNA Microarrays; James Glick¹; Ka Yee Yeung²; Helmut Zarbl³; Paul Vouros¹; ¹Northeastern University, Boston, MA; ²University of Washington, Seattle, WA; ³Robert Wood Johnson Medical School, Piscataway, NJ Proteomic Analysis of a Combined

Melanie Flint^{1,2}; Brian L Hood^{2,4}; Nicolas A 8:30 - 10:30 AM, TUESDAY MORNING Stewart^{3,4}; Mai Sun²; Thomas P. Conrads^{2,4}; ¹Dept ACCURATE MASS LC-MS APPROACHES FOR of Pharmacology & Chemical Biology, CHARACTERIZATION AND QUANTIFICATION OF Pittsburgh, PA; ²Clinical Proteomics Facility, DRUGS AND METABOLITES Pittsburgh, PA; ³Center for Clinical Ballroom B Pharmacology, Pittsburgh, PA; 4University of TOB am 8:30 Identification of a Novel CYP1A2-Mediated Pittsburgh, Pittsburgh, PA **Bioactivation Pathway of Nimesulide Using** MOG pm 4:10 **Investigation of Pharmaceutical and Personal** LTQ-Orbitrap and Q-Trap Mass Care Products in Missouri Natural and Spectrometers; Li Ma; Qian Ruan; Jinping Gan; **Drinking Water Using Liquid** W. Griffith Humphreys; Mingshe Zhu; Bristol-**Chromatography Tandem Mass Spectrometry**; Myers Squibb, Princeton, NJ Yinfa Ma¹; Chuan Wang¹; Sanjeewa TOB am 8:50 Combination of Fast Liquid Chromatography Gamagedara¹; Isaac Stayton¹; Honglan Shi¹; Craig and Quadrupole Time-of-Flight for Adams³; Terry Timmons²; ¹Missouri S&T, Rolla, **Quantitative Analysis of Pharmaceuticals in** MO; ²Missouri Department of natural Resources, Plasma Using Accurate Mass; Gerard Jefferson City, MO; ³University of Kansas, Hopfgartner¹; J.C. Yves Leblanc²; Chantal Lawrence, KS Grivet¹; Emmanuel Varesio¹; ¹University of Geneva, Geneva, Switzerland; ²MDS Analytical 4:45 - 5:30 PM, MONDAY Technologies, Concord, ON AWARD LECTURE An Integrated Approach to in vitro and in vivo TOB am 9:10 Exhibit Hall C Metabolite Quantitation Based on High Recipient of the Award for a Distinguished Contribution in Resolution Full Scan MS Data: Jonathan L. **Mass Spectrometry** Josephs¹: Chiuwa Emily Luk¹: Mary Grubb¹: Yanou Yang¹; Haiying Zhang¹; Hong Cai¹; 8:30 – 10:30 AM, TUESDAY MORNING Robert Langish¹; Petia Shipkova¹; Mark Sanders^{2</SUP; 1}Bristol-Myers Squibb, Pennington, MASS SPECTROMETRY AND BIOFUELS NJ; ²Thermo Fisher Scientific, Somerset, NJ Ballroom A TOB am 9:30 High-Resolution Analysis of the Pyridine-3-TOA am 8:30 Mass Spectrometry in the World of Bioenergy Sulfonyl Derivatives of 17β-Estadiol and its **Research:** An Overview; Mary Lipton; *PNNL*, Metabolites by Orbitrap-Mass Spectrometry; Richland, WA Jacquelyn R. Cole¹; Dmitri Zagorevski²; David C. TOA am 8:50 Biodiesel: Profiling, Stability and MS Spink¹; ¹Wadsworth Center, NYS Department of **Solutions**; G. John Langley¹; Julie Herniman¹; Health, Albany, NY; ²Rensselaer Polytechnic Christianne Wicking¹; Tom Lynch²; ¹University of Institute, Troy, NY Southampton, Southampton, UK; ²BP Castrol TOB am 9:50 2D Mass Mapping: Novel Data Visualization Global Lubricants Technology, Pangbourne, UK Method for Complex Peptide Mixtures TOA am 9:10 Metaproteome Analysis of a Termite Hindgut Analysis; Konstantin Artemenko¹; Alexander R. Microbial Community: Relevant to Biofuel Zubarev¹; Tatiana Samgina²; Albert T. Lebedev²; **Development**; Kristin E Burnum¹; Stephen J Mikhail Savitski¹; Roman Zubarev³; ¹Uppsala Callister¹; Carrie D Nicora¹; Richard D Smith¹; University, Uppsala, Sweden; ²Moscow State Philip Hugenholtz²; Falk Warnecke³; Rudolf H University, Moscow, Russian Federation; Scheffrahn⁴; Mary S Lipton¹; ¹Pacific Northwest ³Karolinska Institute, Stockholm, Sweden National Laboratory, Richland, WA; ²DOE Joint TOB am 10:10 **Method Development for Absolute** Genome Institute, Walnut Creek, CA; ³Lawrence **Quantitation of Insulin Grows Factor Binding** Berkeley National Laboratory, Berkeley, CA; Proteins (IGFBP) in Plasma Samples by ⁴University of Florida, Gainesville, FL Capillary LC-MS; Olaf Boernsen; Denis Herzog; TOA am 9:30 Bio-Char Investigated by Analytical Flash Stephan Charmont; Nelson Guerreiro; Francois Pyrolysis and GCMS; Helge Egsgaard¹; Esben Legay; Stephan Bek; Novartis Pharma AG, Basel, Wilson Bruun¹; Henrik Hauggaard-Nielsen¹; Per Switzerland Ambus¹; Niels Bech²; Norazana Ibrahim²; Peter 8:30 - 10:30 AM, TUESDAY MORNING Arendt Jensen²; ¹Biosystem Division; Risoe-DTU, CHARACTERIZING PROTEIN-LIGAND INTERACTIONS Roskilde, Denmark; ²Department of Chem. Eng; WITH MASS SPECTROMETRY DTU, Lyngby, Denmark Room 201 TOA am 9:50 **Identification of the Extracellular Cellulolytic** TOC am 8:30 Mass Spectrometry-Based Approaches for **Enzymes in Thermophilic Bacteria that Are** Important for Microbial Cellulose Degradation Monitoring Protein-Ligand Interactions: An to Bioethanol; Richard J. Giannone¹; Adriane Overview; Lars Konermann; Jingxi Pan; Brian Lochner¹; Andrew Dykstra^{1,2}; Martin Keller¹; James G. Elkins¹; Robert Hettich¹; ¹Oak Ridge Boys; The University of Western Ontario, London, ON, Canada National Laboratory, Oak Ridge, TN; ²The TOC am 8:50 **Hydroxyl Radical Footprinting of CCL5-**University of Tennessee, Knoxville, TN **Chondroitin Sulfate Complex Reveals both the** TOA am 10:10 Large Array Scheduled MRM Analysis of Binding Interface and a Ligand-Induced Metabolic Pathways Using an Enhanced Scan Conformational Change; Caroline Watson; Fei Rate Hybrid Triple Quadrupole / Linear Ion Yu; James Prestegard; Joshua S. Sharp; Complex Trap; Francesco Pingitore; Sofya Aronova; Carbohydrate Research Center/UGA, Athens, GA

TOC am 9:10

Ligand Binding and Conformational Flexibility

of Ribosomes; William Running; James P. Reilly;

Indiana University, Bloomington, IN

Miryam Kadkhodayan; Guillaume Cottarel;

Codexis, Inc., Redwood City, CA

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TOC am 9:30	Design and Application of Novel Cross-Linking Reagents for Mapping Protein-Protein Interactions; <u>Danielle Vellucci</u> ; Lan Huang; Scott Rychnovsky; <i>University of California</i> , Irvine, CA	TOE am 9:10	Cooley; Nikhil Garge; Benjamin J. Cargile; <u>Maureen K. Bunger</u> ; Research Triangle Institute, Research Triangle Park, NC DIGE/MS and MudPIT: Adaptive Sample Size Re-Estimation to Combine Statistical
TOC am 9:50	Investigation of VDR Modulator Interactions with the Full Length VDR/RXRα Nuclear Receptor Complex by HDX-MS; Jun Zhang; Michael Chalmers; Bruce Pascal; Patrick Griffin; The Scripps Research Institute, Scripps Florida,	TOE am 9:30	Power with Depth of Coverage; W. Hayes Mcdonald; Bing Zhang; Lillian B. Nanney; David B. Friedman; Vanderbilt University School of Medicine, Nashville, TN Relative Quantitative Analyses of Intact
TOC am 10:10	Jupiter, FL Thermodynamic Analysis of Chaperone- Substrate Complexes; Ying Xu ¹ ; Sebastian Schmitt ² ; Liangjie Tang ³ ; Ursula Jakob ² ; Michael C. Fitzgerald ¹ ; Juke University, Durham, NC;	102 um 7.30	Methylated Yeast Ribosomal Proteins Using Fourier-Transform Mass Spectrometry; Kristofor Webb; Rebecca Lipson; Julian Whitelegge; Steven Clarke; University of California Los angeles, Los Angeles, CA
	² University of Michigan, Ann Arbor, MI; ³ ExSAR Corporation, Monmouth Junction, NJ	TOE am 9:50	A New Realm for Protein Quantitation: Reproducibility and Modification Occupancy
NOVEL DEV	0 – 10:30 AM, TUESDAY MORNING VELOPMENTS IN MASS SPECTROMETRY TRUMENTATION: ION SOURCES Room 204		Using Label-Free Top Down Mass Spectrometry; John F. Kellie ¹ ; Ji Eun Lee ¹ ; John C. Tran ¹ ; Dorothy R. Ahlf ¹ ; Haylee M. Thomas ¹ ; Adaickalam Vellaichamy ¹ ; Jeremiah D. Tipton ² ;
TOD am 8:30	Infrared Matrix-Assisted Laser Desorption Electrospray Ionization Coupled to FT-ICR Mass Spectrometry; Kermit K. Murray ¹ ; Jason S. Sampson ² ; David C. Muddiman ² ; ¹ Louisiana	TOE am 10:10	Alan G. Marshall ^{2,3} ; Neil L; ¹ University of Illinois, Urbana, IL; ² National High Magnetic Field Laboratory, Tallahassee, FL; ³ Florida State University, Tallahassee, FL Differential Gel Electrophoresis Examination
TOD am 8:50	State Univ., Baton Rouge, LA; ² North Carolina State University, Raleigh, NC Desorption Electrospray/Metastable-Induced Ionization (DEMI): A New Ambient Multimode Ionization Technique; Leonard Nyadong; Asiri Galhena; <u>Facundo Fernandez</u> ;		of Asian Ash Tree Resistance to Emerald Ash Borer Attack Verses North American Ash Tree Susceptibility; Kari Green-church; Alexandra Popoval-Butler; Cindy James; Justin GA Whitehill; Nan M Kleinholz; Daniel A. Herms;
TOD am 9:10	Georgia Institute of Technology, Atlanta, GA Enhanced Control of Nanophotonic Ion		Pierluigi Bonello; The Ohio State University, Columbus, OH
	Production by Laser Desorption Ionization	8:30	0 – 10:30 AM, TUESDAY MORNING
	from Tailored Nanopost Arrays; <u>Jessica A.</u> <u>Stolee</u> ¹ ; Bennett N. Walker ¹ ; Deanna L. Pickel ² ;		S-PHASE METAL ION CHEMISTRY Room 103
	from Tailored Nanopost Arrays; Jessica A. Stolee ¹ ; Bennett N. Walker ¹ ; Deanna L. Pickel ² ; Scott Retterer ² ; Akos Vertes ¹ ; ¹ George Washington University, Washington, DC; ² Oak	TOF am 8:30	Room 103 Gas-Phase Reactions of Transition Metal Complexes with Diazoacetates: Substituent
TOD am 9:30	from Tailored Nanopost Arrays; Jessica A. Stolee¹; Bennett N. Walker¹; Deanna L. Pickel²; Scott Retterer²; Akos Vertes¹; ¹George Washington University, Washington, DC; ²Oak Ridge National Laborator, Oak Ridge, TN Implementation of an EI/CI Interface on a Hybrid Orbitrap System for Ultra-High Resolution GC-MS; Amelia C. Peterson; Graeme	TOF am 8:30	Room 103 Gas-Phase Reactions of Transition Metal Complexes with Diazoacetates: Substituent Effects and the Formation of Novel Organometallic Species; Scott Gronert; Scott K. Koehn; Virginia Commonwealth Uni, Richmond, VA
	from Tailored Nanopost Arrays; Jessica A. Stolee ¹ ; Bennett N. Walker ¹ ; Deanna L. Pickel ² ; Scott Retterer ² ; Akos Vertes ¹ ; ¹ George Washington University, Washington, DC; ² Oak Ridge National Laborator, Oak Ridge, TN Implementation of an EI/CI Interface on a Hybrid Orbitrap System for Ultra-High Resolution GC-MS; Amelia C. Peterson; Graeme C. McAlister; Joshua J. Coon; University of Wisconsin, Madison, WI		Room 103 Gas-Phase Reactions of Transition Metal Complexes with Diazoacetates: Substituent Effects and the Formation of Novel Organometallic Species; Scott Gronert; Scott K. Koehn; Virginia Commonwealth Uni, Richmond, VA Competition between Cluster Fragmentation, C-C Bond Coupling and C-X Bond Activation
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TOD am 9:50 TOD am 10:10	from Tailored Nanopost Arrays; Jessica A. Stolee¹; Bennett N. Walker¹; Deanna L. Pickel²; Scott Retterer²; Akos Vertes¹; ¹George Washington University, Washington, DC; ²Oak Ridge National Laborator, Oak Ridge, TN Implementation of an EI/CI Interface on a Hybrid Orbitrap System for Ultra-High Resolution GC-MS; Amelia C. Peterson; Graeme C. McAlister; Joshua J. Coon; University of Wisconsin, Madison, WI Towards Total Ion Utilization: Electrospray Ionization in a Sub-Ambient Pressure Environment for High Sensitivity Mass Spectrometry; Jason Page; Ioan Marginean; Ryan Kelly; Keqi Tang; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA Plasma-based Ambient Desorption/Ionization Mass Spectrometry (ADI-MS): Investigations into Desorption Characteristics and Competitive Ionization; Jacob T. Shelley; Kevin P. Pfeuffer; Steven J. Ray; Gary M. Hieftje; Indiana University, Bloomington, IN	TOF am 8:30	Gas-Phase Reactions of Transition Metal Complexes with Diazoacetates: Substituent Effects and the Formation of Novel Organometallic Species; Scott Gronert; Scott K. Koehn; Virginia Commonwealth Uni, Richmond, VA Competition between Cluster Fragmentation, C-C Bond Coupling and C-X Bond Activation in Silver Hexynyl Cluster Cations, [(C4H9CCAg)nAg]+. Size Does Matter! Richard A. J. O'hair¹; Farrah Q Wang¹.²; George N. Khairallah¹.²; Craig M Williams⁴; George Koutsantonis³,¹ University of Melbourne, Victoria, Australia; ²Bio21 Inst, Uni of Melbourne, Melbourne, Australia; ³University of Western Australia, Perth, Australia; ⁴University of Queensland, Brisbane, Australia Hydration Energies and Charge Separation Processes of Group 12 Dications; Theresa Cooper; Damon R Carl; Peter B. Armentrout; University of Utah, Department of Chemistry, Salt
TOD am 9:50 TOD am 10:10	from Tailored Nanopost Arrays; Jessica A. Stolee¹; Bennett N. Walker¹; Deanna L. Pickel²; Scott Retterer²; Akos Vertes¹; Jeorge Washington University, Washington, DC; Joak Ridge National Laborator, Oak Ridge, TN Implementation of an EI/CI Interface on a Hybrid Orbitrap System for Ultra-High Resolution GC-MS; Amelia C. Peterson; Graeme C. McAlister; Joshua J. Coon; University of Wisconsin, Madison, WI Towards Total Ion Utilization: Electrospray Ionization in a Sub-Ambient Pressure Environment for High Sensitivity Mass Spectrometry; Jason Page; Ioan Marginean; Ryan Kelly; Keqi Tang; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA Plasma-based Ambient Desorption/Ionization Mass Spectrometry (ADI-MS): Investigations into Desorption Characteristics and Competitive Ionization; Jacob T. Shelley; Kevin P. Pfeuffer; Steven J. Ray; Gary M. Hieftje;	TOF am 8:30 TOF am 8:50	Gas-Phase Reactions of Transition Metal Complexes with Diazoacetates: Substituent Effects and the Formation of Novel Organometallic Species; Scott Gronert; Scott K. Koehn; Virginia Commonwealth Uni, Richmond, VA Competition between Cluster Fragmentation, C-C Bond Coupling and C-X Bond Activation in Silver Hexynyl Cluster Cations, [(C4H9CCAg)nAg]+. Size Does Matter! Richard A. J. O'hair¹; Farrah Q Wang¹,²; George N. Khairallah¹,²; Craig M Williams⁴; George Koutsantonis³; University of Melbourne, Victoria, Australia; Bio21 Inst, Uni of Melbourne, Melbourne, Australia; University of Western Australia, Perth, Australia; University of Queensland, Brisbane, Australia Hydration Energies and Charge Separation Processes of Group 12 Dications; Theresa Cooper; Damon R Carl; Peter B. Armentrout; University of Utah, Department of Chemistry, Salt Lake City, UT Connecting Reduction Energies of Hydrated Metal Ions to Aqueous Solution: The Absolute
TOD am 9:50 TOD am 10:10	from Tailored Nanopost Arrays; Jessica A. Stolee¹; Bennett N. Walker¹; Deanna L. Pickel²; Scott Retterer²; Akos Vertes¹; ¹George Washington University, Washington, DC; ²Oak Ridge National Laborator, Oak Ridge, TN Implementation of an EI/CI Interface on a Hybrid Orbitrap System for Ultra-High Resolution GC-MS; Amelia C. Peterson; Graeme C. McAlister; Joshua J. Coon; University of Wisconsin, Madison, WI Towards Total Ion Utilization: Electrospray Ionization in a Sub-Ambient Pressure Environment for High Sensitivity Mass Spectrometry; Jason Page; Ioan Marginean; Ryan Kelly; Keqi Tang; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA Plasma-based Ambient Desorption/Ionization Mass Spectrometry (ADI-MS): Investigations into Desorption Characteristics and Competitive Ionization; Jacob T. Shelley; Kevin P. Pfeuffer; Steven J. Ray; Gary M. Hieftje; Indiana Univeristy, Bloomington, IN D-10:30 AM, TUESDAY MORNING ITATIVE INTACT PROTEOMICS (QIP)	TOF am 8:30 TOF am 8:50 TOF am 9:10	Gas-Phase Reactions of Transition Metal Complexes with Diazoacetates: Substituent Effects and the Formation of Novel Organometallic Species; Scott Gronert; Scott K. Koehn; Virginia Commonwealth Uni, Richmond, VA Competition between Cluster Fragmentation, C-C Bond Coupling and C-X Bond Activation in Silver Hexynyl Cluster Cations, [(C4H9CCAg)nAg]+. Size Does Matter! Richard A. J. O'hair'; Farrah Q Wang ^{1,2} ; George N. Khairallah ^{1,2} ; Craig M Williams ⁴ ; George Koutsantonis ³ ; University of Melbourne, Victoria, Australia; Bio21 Inst, Uni of Melbourne, Melbourne, Australia; University of Western Australia, Perth, Australia; University of Queensland, Brisbane, Australia Hydration Energies and Charge Separation Processes of Group 12 Dications; Theresa Cooper; Damon R Carl; Peter B. Armentrout; University of Utah, Department of Chemistry, Salt Lake City, UT Connecting Reduction Energies of Hydrated

1 age 514			37 ASIMB Conference on Mass Spectrometry
TOF am 10:10	Complexes under Activation Conditions; Francoise Fournier; Carlos Afonso; Denis Lesage; Valérie Mancel; Nicole Sellier; <u>Jean-Claude</u> <u>Tabet</u> ; <i>University Paris VI (UPMC), Paris Cedex O5, France</i> Radical Cations of Methionine, α- Methylmethionine and S-Methylcysteine: Generations and Dissociations in the Gas Phase; <u>Junfang Zhao</u> ¹ ; Dominic C. M. Ng ² ; Ivan K. Chu ² ; A.C. Hopkinson ¹ ; K W Michael Siu ¹ ; ¹ York University, Toronto, Canada; ² University of Hong Kong, Hongkong, China	TOA pm 3:10	Zhang¹; Wenying Li¹; Weiping Zhao³; Jonathan L. Josephs²⁴; william humphreys¹; Mingshe Zhu⁵; ¹Bristol-Myers Squibb R&D, Pennington, NJ; ²Bristol-Myers Squibb, Princeton, NJ; ³Bristol Myers Squibb, Princeton, NJ; ⁴Bristol-Myers Squibb, Pennington, NJ; ⁵Bristol-Myers Squibb, Princeton, NJ Metabolite Profiling Challenges in the First-in-Human Study. Identification of Two Novel Metabolites of a Nociceptin Agonist; Natalia Penner¹; Swapan K. Chowdhury²; ¹Biogen Idec, Cambridge, MA; ²Schering-Plough, Kenilworth,
	– 10:30 AM, TUESDAY MORNING		NJ
MASS SPEC	FROMETRY IN HOMELAND PROTECTION	TOA pm 3:30	A Review of Accurate Mass LC-MS
	Room 113		Applications for Compliance with MIST
TOG am 8:30	Mass Spectrometry in Biodefense; Catherine		Guidelines; Richard Clayton; Brian Morrison;
100 um 0.50	Fenselau; <i>University of Maryland, College Park</i> ,		John Kendrick; Covance Laboratories, Ltd,
			Harrogate, North Yorkshire, UK
TOC 0.50	MD	TOA pm 3:50	A Retention-Time-Shift-Tolerant Background-
TOG am 8:50	Mass Spectrometric Tools to Determine Ricin	10/1 pm 3.30	e
	Sample Processing Methods; Karen L. Wahl;		Subtraction and Noise-Reduction Algorithm
	Helen W. Kreuzer-Martin; Jon H. Wahl; Heather		(BgS-NoRA) for Extraction of Drug
	A. Colburn; David S. Wunschel; Brian H.		Metabolites in LC-MS Data; Peijuan Penny
	Clowers; Pacific Northwest National Laboratory,		Zhu; Wei Ding; Wei Tong; Anima Ghosal; Kevin
	Richland, WA		Alton; Swapan K. Chowdhury; Schering-Plough
TOG am 9:10	Rapid Detection of Botulinum Neurotoxin in a		Research Institute, Kenilworth, NJ
100 am 7.10	Spiked Sample through Activity Detection and	TOA pm 4:10	Rapid Detection and Characterization of N-
		•	acetyl-L-Cysteine Conjugates in Human Urine
	Proteomics; Suzanne R. Kalb ¹ ; Hercules Moura ¹ ;		Using Polarity Switching of Quadrupole-
	Theresa J. Smith ² ; Leonard A. Smith ² ; James D.		Linear Ion Trap Mass Spectrometry; Wenying
	Marks ³ ; John R. Barr ¹ ; ¹ CDC, Atlanta, GA;		Jian ¹ ; Ming Yao ² ; Duxi Zhang ² ; Mingshe Zhu ² ;
	² USAMRIID, Ft. Detrick, MD; ³ University of		Jan , Willig 1 ao , Duxi Zhang , Willigshe Zhu , Johnson and Johnson, Raritan, NJ; ² Bristol-
	California at San Francisco, San Francisco, CA		
TOG am 9:30	Rapid Identification of E. coli O157:H7 by		Myers Squibb, Princeton, NJ
	"Top-Down" Proteomics Using MALDI-		– 4:30 PM, TUESDAY AFTERNOON
	TOE/TOE Many Connections of the Clifford V	CA	AALI MOLECIILE DIOMADIZEDE
	TOF/TOF Mass Spectrometry; Clifton K.	51	MALL MOLECULE BIOMARKERS
			Ballroom B
	<u>Fagerquist</u> ¹ ; Brandon R. Garbus ¹ ; Katherine E.		Ballroom B
	<u>Fagerquist</u> ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ;	TOB pm 2:30	Ballroom B Exposure and Response Biomarkers of
	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E.		Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary
	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <8; ¹ USDA, ARS, Albany, CA; ² UCSF,		Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L.
TOG am 0:50	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ Si JUSDA, ARS, Albany, CA; ² UCSF, Department of Medicine, San Francisco, CA		Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of
TOG am 9:50	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ^{1USDA, ARS, Albany, CA, ²UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass}	TOB pm 2:30	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA
TOG am 9:50	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ Mandrell ¹ Si USDA, ARS, Albany, CA; ² UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker		Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of
TOG am 9:50	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <'S; ¹ USDA, ARS, Albany, CA; ² UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin	TOB pm 2:30	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a
TOG am 9:50	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ Mandrell¹ JUSDA, ARS, Albany, CA; ²UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki	TOB pm 2:30	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe ¹ ; Barry S
	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ Mandrell¹ JUSDA, ARS, Albany, CA; ²UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ	TOB pm 2:30	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹;
TOG am 9:50 TOG am 10:10	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <8; IUSDA, ARS, Albany, CA, ² UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion	TOB pm 2:30	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹;
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	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <8; IUSDA, ARS, Albany, CA; IUCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes ¹ ; Michael P. Tolocka ¹ ; Kermit K. Murray ¹ ; Ernest K. Lewis ² ; Thomas Egan ² ; J. Albert	TOB pm 2:30 TOB pm 2:50	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH
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	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <8; IUSDA, ARS, Albany, CA; IUCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes ¹ ; Michael P. Tolocka ¹ ; Kermit K. Murray ¹ ; Ernest K. Lewis ² ; Thomas Egan ² ; J. Albert Schultz ² ; ILouisiana State University, Baton	TOB pm 2:30 TOB pm 2:50	Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe ¹ ; Barry S Lutzke ¹ ; Angela S Freeman ¹ ; Susan E Pratt ¹ ; Angela Bones ¹ ; Crystal A Dotson-Roberts ¹ ; Bradley L. Ackermann ¹ ; Anne H Dantzig ¹ ;; ¹ Eli Lilly and Company, Indianapolis, IN; ² The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue
	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ Mandrell¹ Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes¹; Michael P. Tolocka¹; Kermit K. Murray¹; Ernest K. Lewis²; Thomas Egan²; J. Albert Schultz²; ¹Louisiana State University, Baton Rouge, LA; ²Ionwerks Inc., Houston, TX	TOB pm 2:30 TOB pm 2:50	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones;
	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <8; IUSDA, ARS, Albany, CA; IUCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes ¹ ; Michael P. Tolocka ¹ ; Kermit K. Murray ¹ ; Ernest K. Lewis ² ; Thomas Egan ² ; J. Albert Schultz ² ; ILouisiana State University, Baton	TOB pm 2:30 TOB pm 2:50	Ballroom B Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones; Jeffrey C. Hanson²; Donald Johann³; Jaime
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	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ¹ <8; ¹ USDA, ARS, Albany, CA; ² UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes ¹ ; Michael P. Tolocka ¹ ; Kermit K. Murray ¹ ; Ernest K. Lewis ² ; Thomas Egan ² ; J. Albert Schultz ² ; ¹ Louisiana State University, Baton Rouge, LA; ² Ionwerks Inc., Houston, TX	TOB pm 2:30 TOB pm 2:50	Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones; Jeffrey C. Hanson²; Donald Johann³; Jaime Rodriguez-Canales²; Xia Xu¹; Josip Blonder¹; Michael R. Emmert-Buck²; Timothy D.
TOG am 10:10	Fagerquist ¹ ; Brandon R. Garbus ¹ ; Katherine E. Williams ² ; Anna H. Bates ¹ ; Siobhan Boyle ¹ ; Leslie A. Harden ¹ ; William G. Miller ¹ ; Robert E. Mandrell ^{1-(S); 1} USDA, ARS, Albany, CA; ² UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes ¹ ; Michael P. Tolocka ¹ ; Kermit K. Murray ¹ ; Ernest K. Lewis ² ; Thomas Egan ² ; J. Albert Schultz ² ; ¹ Louisiana State University, Baton Rouge, LA; ² Ionwerks Inc., Houston, TX 10:30 AM – 2:30 PM, TUESDAY POSTER SESSION Exhibit Hall AB	TOB pm 2:30 TOB pm 2:50	Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones; Jeffrey C. Hanson²; Donald Johann³; Jaime Rodriguez-Canales²; Xia Xu¹; Josip Blonder¹;
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TOG am 10:10 2:30 LC-MS ASS COM	Fagerquist¹; Brandon R. Garbus¹; Katherine E. Williams²; Anna H. Bates¹; Siobhan Boyle¹; Leslie A. Harden¹; William G. Miller¹; Robert E. Mandrell¹ Mandrell¹ Yold ARS, Albany, CA; ²UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes¹; Michael P. Tolocka¹; Kermit K. Murray¹; Ernest K. Lewis²; Thomas Egan²; J. Albert Schultz²; ¹Louisiana State University, Baton Rouge, LA; ²Ionwerks Inc., Houston, TX 10:30 AM − 2:30 PM, TUESDAY POSTER SESSION Exhibit Hall AB -4:30 PM, TUESDAY AFTERNOON SESSMENT OF HUMAN METABOLISM IN PLIANCE WITH "MIST" GUIDANCE Ballroom A A New Paradigm for Metabolite Profiling and Bioanalysis to Identify and Manage Metabolite Safety Concerns; Scott W. Grimm; AstraZeneca Pharmaceuticals, Wilmington, DE A Methodology for Complete Plasma	TOB pm 2:30 TOB pm 2:50 TOB pm 3:10	Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones; Jeffrey C. Hanson²; Donald Johann³; Jaime Rodriguez-Canales²; Xia Xu¹; Josip Blonder¹; Michael R. Emmert-Buck²; Timothy D. Veenstra¹; ¹SAIC-Frederick, Inc., Frederick, MD; ²National Cancer Institute, Bethesda, MD; ³NIH, Bethesda, MD Metabolic Biomarkers Discovery; Vladimir Tolstikov; UC Davis Genome Center, Davis, CA High Throughput UFLC-MS/MS Analysis of Urinary Prostanoids before and after Exercise; Matt Blatnik¹; Rick Steenwyk²; ¹Pfizer Inc., Groton, CT; ²Pfizer, Lebanon, CT Mass Spectrometry Strategies for Lipidome
2:30 LC-MS ASS COM TOA pm 2:30	Fagerquist¹; Brandon R. Garbus¹; Katherine E. Williams²; Anna H. Bates¹; Siobhan Boyle¹; Leslie A. Harden¹; William G. Miller¹; Robert E. Mandrell¹ Mandrell¹ Mandrell¹ I USDA, ARS, Albany, CA; ²UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes¹; Michael P. Tolocka¹; Kermit K. Murray¹; Ernest K. Lewis²; Thomas Egan²; J. Albert Schultz²; ¹Louisiana State University, Baton Rouge, LA; ²Ionwerks Inc., Houston, TX 10:30 AM − 2:30 PM, TUESDAY POSTER SESSION Exhibit Hall AB -4:30 PM, TUESDAY AFTERNOON SESSMENT OF HUMAN METABOLISM IN PLIANCE WITH "MIST" GUIDANCE Ballroom A A New Paradigm for Metabolite Profiling and Bioanalysis to Identify and Manage Metabolite Safety Concerns; Scott W. Grimm; AstraZeneca Pharmaceuticals, Wilmington, DE A Methodology for Complete Plasma Metabolite Profiling and Identification with	TOB pm 2:30 TOB pm 2:50 TOB pm 3:10 TOB pm 3:30 TOB pm 3:50	Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones; Jeffrey C. Hanson²; Donald Johann³; Jaime Rodriguez-Canales²; Xia Xu¹; Josip Blonder¹; Michael R. Emmert-Buck²; Timothy D. Veenstra¹; ¹SAIC-Frederick, Inc., Frederick, MD; ²National Cancer Institute, Bethesda, MD; ³NIH, Bethesda, MD Metabolic Biomarkers Discovery; Vladimir Tolstikov; UC Davis Genome Center, Davis, CA High Throughput UFLC-MS/MS Analysis of Urinary Prostanoids before and after Exercise; Matt Blatnik¹; Rick Steenwyk²; ¹Pfizer Inc., Groton, CT; ²Pfizer, Lebanon, CT Mass Spectrometry Strategies for Lipidome Analysis and the Identification of Lipid
2:30 LC-MS ASS COM TOA pm 2:30	Fagerquist¹; Brandon R. Garbus¹; Katherine E. Williams²; Anna H. Bates¹; Siobhan Boyle¹; Leslie A. Harden¹; William G. Miller¹; Robert E. Mandrell¹ Mandrell¹ Yold ARS, Albany, CA; ²UCSF, Department of Medicine, San Francisco, CA The Use of Affinity Capture Mass Spectrometry for Detection of Biomarker Proteins and Biological Warfare Agents; Erin Johnson; Walther Ellis; Linda Powers; Vicki Wysocki; University of Arizona, Tucson, AZ Bioaerosol Detection Using MALDI Ion Mobility and Mass Spectrometry; Juaneka M. Hayes¹; Michael P. Tolocka¹; Kermit K. Murray¹; Ernest K. Lewis²; Thomas Egan²; J. Albert Schultz²; ¹Louisiana State University, Baton Rouge, LA; ²Ionwerks Inc., Houston, TX 10:30 AM − 2:30 PM, TUESDAY POSTER SESSION Exhibit Hall AB -4:30 PM, TUESDAY AFTERNOON SESSMENT OF HUMAN METABOLISM IN PLIANCE WITH "MIST" GUIDANCE Ballroom A A New Paradigm for Metabolite Profiling and Bioanalysis to Identify and Manage Metabolite Safety Concerns; Scott W. Grimm; AstraZeneca Pharmaceuticals, Wilmington, DE A Methodology for Complete Plasma	TOB pm 2:30 TOB pm 2:50 TOB pm 3:10 TOB pm 3:30 TOB pm 3:50	Exposure and Response Biomarkers of Cigarette Smoke: Implications in Pulmonary Disease Onset and Progression; Stacy L. Gelhaus; Ian A. Blair; Univ. of Penn/SOM/Pharmacol, Philadelphia, PA Understanding the Incorporation of Gemcitabine into DNA and its Application as a Biomarker; Enaksha R Wickremsinhe¹; Barry S Lutzke¹; Angela S Freeman¹; Susan E Pratt¹; Angela Bones¹; Crystal A Dotson-Roberts¹; Bradley L. Ackermann¹; Anne H Dantzig¹;; ¹Eli Lilly and Company, Indianapolis, IN; ²The Cleveland Clinic, Cleveland, OH Determining the Compatibility between Processing and Staining Methods for Histological Analysis of Frozen Tissue Specimens and LC-MS Analysis of Hormones; Jeffrey C. Hanson²; Donald Johann³; Jaime Rodriguez-Canales²; Xia Xu¹; Josip Blonder¹; Michael R. Emmert-Buck²; Timothy D. Veenstra¹; ¹SAIC-Frederick, Inc., Frederick, MD; ²National Cancer Institute, Bethesda, MD; ³NIH, Bethesda, MD Metabolic Biomarkers Discovery; Vladimir Tolstikov; UC Davis Genome Center, Davis, CA High Throughput UFLC-MS/MS Analysis of Urinary Prostanoids before and after Exercise; Matt Blatnik¹; Rick Steenwyk²; ¹Pfizer Inc., Groton, CT; ²Pfizer, Lebanon, CT Mass Spectrometry Strategies for Lipidome

Busik; Gavin E. Reid; Michigan State University, East Lansing, MI

2:30 – 4:30 PM, TUESDAY AFTERNOON ADVANCES IN THE CHARACTERIZATION OF GLYCOPROTEINS

Room 201

TOC pm 2:30 A Lectin Affinity-Based Biomarker Discovery
Workflow Targeting Cancer-Specific
Glycopeptides in Human Plasma; Penelope M.
Drake²; Eric Johansen²; Richard Niles²; Michael
Lerch²; Haichuan Liu²; Bensheng Li⁵; Simon
Allen²; Kwanyoung Jung⁶; Steven C. Hall²; Bir;

¹Buck Inst. for Age Research, Novato, CA; ²UCSF
Mass Spectrometry Core, San Francisco, CA;

³Buck Institute for Age Research, Novato, CA;

⁴UC San Francisco, San Francisco, CA; ⁵Buck
Inst for Age Research

TOC pm 2:50

In-Depth Urinary N-Glycoproteome Profiling in Normal and Prostate Cancer Patient Urine; Yong Zhou¹; Laura Knutzen¹; Hector Ramos¹; Carey Sheu¹; Paul Shannon¹; Hui Zhang²; Julian D Watts¹; Alvin Liu³; Ruedi Aebersold^{1,4};

¹Institute for Systems Biology, Seattle, WA; ²Johns Hopkins Medical Institutions, Baltimore, MD;

³University of Washington School of Medicine, Seattle, WA; ⁴IMBS, ETH&Faculty of Science, U of Zurich, Switzerland

TOC pm 3:10 Glycopeptide Analysis of HIV-1 Envelope
Proteins: Influence of Glycosylation on
Envelope Immunogenicity; Eden P. Go¹; Qing
Chang¹; Hua-Xin Liao²; Sutherland Laura²; Munir
Alam²; Barton F. Haynes²; Heather Desaire¹;

¹University of Kansas, Lawrence, KS; ²Duke
University Medical Center, Durham, NC

TOC pm 3:30 Glycomics of the Antibacterial Salivary
Agglutinin Protein Using LC-MS; Niclas G.
Karlsson¹; Samah Issa¹; Antoon J.M. Ligtenberg²;

School of Chemistry, NUI Galway, Galway,
Ireland; Department of Oral Biochemistry, Free
University, Amsterdam, The Netherlands

TOC pm 3:50

Site-Specific Glycosylation of Human Serum
Glycoproteins via Partition and Quantitation of
the N-Glycome-Utility for Disease Biomarker
Discovery; Caroline S. Chu¹; Ning Tang²; John
Froehlich¹; Tony Ferrige³; Robert Alecio⁴; Patrick
D. Perkins²; Kevin Killeen⁵; Keith Waddell²;
Rudolf Grimm²
Rudolf Grimm²
JUC Davis, Davis, CA; ²Agilent
Technologies, Santa Clara, CA; ³Positive
Probability Limited, Ely, UK; ⁴Positive
Probability Ltd, Sittingbourne, UK; ⁵Agilent
Laboratories, Santa

TOC pm 4:10

Identification and Quantitation of
Phosphorylated and O-GlcNAcylated Proteins
Associated with Mitotic Spindles and
Midbodies during Cytokinesis (Part B);
Namrata Udeshi¹, Zihao Wang²; Chad Slawson²;
Philip Compton¹; Jeffrey Shabanowitz¹; Gerald
W. Hart²; Donald F. Hunt¹, ¹University of
Virginia, Charlottesville, VA; ²Johns Hopkins
School of Medicine, Baltimore, MD

2:30 – 4:30 PM, TUESDAY AFTERNOON NOVEL DEVELOPMENTS IN MASS SPECTROMETRY INSTRUMENTATION: ANALYZERS, DETECTORS, TANDEM INSTRUMENTS Room 204

TOD pm 2:30 A High Mass Resolution, Multiplexed Time-of-Flight Mass Spectrometer; Robert H. Jackson; Zhongyu Yang; C. Bronson Crothers; David A. Ferris; <u>Stephen A. Lammert</u>; *Stillwater Scientific Instruments, Inc., Orono, ME*

TOD pm 2:50 Direct Analysis Of Neutrals Using
Superconducting Detector in Tandem Mass
Spectrometry; Masataka Ohkubo¹; Masahiro
Ukibe¹; Shigetomo Shiki¹; Shigeo Tomita²;
Shigeo Hayakawa³; ¹National Inst. of Adv. Indust.
Sci. Tech. (AIST), Tsukuba, Ibaraki; ²University
of Tsukuba, Tsukuba, Ibaraki; ³Osaka Prefecture
University, Sakai, Osaka

TOD pm 3:10 Comparison of As-Built and Simion®
Model Results for a Toroidal Ion Trap Mass
Spectrometer; Joseph Oliphant; Edgar Lee; Eric
Handberg; Torion Technologies, Inc., American
Fork, UT

TOD pm 3:30

Increased Proteome Definition Exploiting
Performance Enhancements of a New Linear
Ion Trap Mass Spectrometer; Tonya P. Second;
Justin Blethrow; Vlad Zabrouskov; Jae C.
Schwartz; Thermo Fisher Scientific, San Jose, CA
TOD pm 3:50

Ion-Ion Interactions in the Orbitrap Mass

Ion-Ion Interactions in the Orbitrap Mass
Analyzer; Richard H. Perry¹; Gary Abdiel
Salazar¹; Qizhi Hu²; R. Graham Cooks¹; Robert J.
Noll¹; Purdue University, West Lafayette, IN;
²Amgen, Inc., Thousand Oaks, CA

TOD pm 4:10 Multiple-Reflection Time-of-Flight Mass
Spectrometry of Exotic Nuclei; Wolfgang R.

Plass^{1,2}; Timo Dickel²; Arno Becker²; Ulrich
Czok²; Hans Geissel^{1,2}; Christian Jesch²; Wadim
Kinsel^{1,2}; Martin Petrick^{1,2}; Katrin Reinheimer^{2</;}

IGSI, Darmstadt, Germany; Justus-LiebigUniversitaet Giessen, Giessen, Germany;

Institute for Analytical Instrumentation, St.
Petersburg, Russia

2:30 – 4:30 PM, TUESDAY AFTERNOON THE ROLE OF MASS SPECTROMETRY IN UNDERSTANDING CELLULAR PATHWAYS Exhibit Hall C

TOE pm 2:30

Quantitative Phosphoproteomics Identifies
Sites in K-Cl Cotransporters that Regulate Cell
Volume and Neuronal Excitation; Jesse
Rinehart¹; Yelena D. Maksimova¹; Jessica E.
Tanis¹; Kathy Stone¹; Junhui Zhang¹; Mary
Risinger³; Weijun Pan¹; Dianqing Wu¹;
Christopher Colangelo<S; ¹Yale University, New
Haven, CT; ²Howard Hughes Medical Institute,
New Haven, CT; ³University of Cincinnati
College of Medicine, Cincinnati, OH

TOE pm 2:50 A Targeted Spatial-Temporal Proteomic
Approach Reveals New Cellular Pathways
Involved in Human Cytomegalovirus Virion
Maturation; Nathaniel J. Moorman; Thomas E.
Shenk; Ileana M. Cristea; Princeton University,
Princeton, NJ

TOE pm 3:10 Lysine Butyrylation is a Prevalent and Evolutionarily-conserved Posttranslational Modification Pathway; Zhongyi Cheng; Kai Zhang; Zhihong Zhang; Yue Chen; Minjia Tan; Yingming Zhao; University of Chicago, Chicago,

TOE pm 3:30 Mapping Epigenetic Signaling Networks (the Human Epigenome) Using a Combined Proteomic-Genomic Approach; Gary LeRoy; Nicolas L. Young; Mariana D. Plazas-Mayorca; Benjamin A. Garcia; Princeton University, Princeton, NJ

Pa	ge	S	1	6

Page S16			57" ASMS Conference on Mass Spectrometry
TOE pm 3:50 TOE pm 4:10	Toward Simultaneously Assessing the Activation State of the Kinome including Substrate-Kinase Relationship; Kazuishi Kubota ¹ ; Rana Anjum ¹ ; Yonghao Yu ¹ ; Adam Feldman ² ; Chin-Lee Wu ² ; John Rush ³ ; Judit Villen ¹ ; Steven Gygi ¹ ; Harvard Medical School, Boston, MA; Massachusetts General Hospital, Boston, MA; Cell Signaling Technology, Danvers, MA Proteomics «Google»-Like Tool for Signaling Pathways; Roman Zubarev; Konstantin Artemenko; Corina Mayrhofer; Y.M. Eva Fung; Karolinska Institute, Stockholm, Sweden	TOG pm 3:50	Protein by Solution-Phase H/D Exchange FT-ICR Mass Spectrometry; Hui-Min Zhang¹; Shaun Mcloughlin²; Huan He¹; Carol Nilsson³; Mark R. Emmett¹; Alan G. Marshall¹; 'Nat'l High Magnetic Field Lab/Florida State Univ., Tallahassee, FL; ²Abbott Laboratories, Abbott Park, IL; ³Pfizer, Inc., San Diego, CA Amyloidogenic beta-2-Microglobulin Transiently Populates a Long-Lived Unfolded State; Thomas J.d. Jorgensen¹; Lei Cheng²; Anna Jansson⁴; Niels H.H. Heegaard³; ¹University of Southern Denmark, Odense M, Denmark; ²Dept. Biochemistry & Molecular Biology, Odense M,
2:30	0 – 4:30 PM, TUESDAY AFTERNOON		Denmark; ³ Statens Serum Institut, Copenhagen,
	TERS/COMPLEXES/SOLVATED IONS		Denmark; ⁴ Sidec AB, Stockholm, Sweden
	Room 103	TOG pm 4:10	Examination of Electron-Induced
TOF pm 2:30 TOF pm 2:50	Characterization of Floppy Systems with Vibrational Spectroscopy: Learning to Live with Anharomic Effects; Mark Johnson; Yale University, New Haven, CT Hydration of Hydrophobic and High Charge State Ions: Transitions from Gas-Phase		Fragmentation of Intact Protein Ions as a New Tool in Top-Down HDX MS Measurements; Rinat Abzalimov ¹ ; Desmond Kaplan ² ; Michael Easterling ² ; Igor A. Kaltashov ¹ ; ¹ University of Massachusetts, Amherst, MA; ² Bruker Daltonics, Inc., Billerica, MA
	Structure to Bulk; James Prell; Jeremy T		A AF . F 30 DM FILEOD AN
	O'Brien; Evan R. Williams; University of		4:45 – 5:30 PM, TUESDAY AWARD LECTURE
TOF 2.10	California, Berkeley, CA Structures of Hydrated Metalated and Proton-		Exhibit Hall C
TOF pm 3:10	Bound Dimer Adenine by IRMPD	4:45 pm	Presentation of the Thermo Scientific
	Spectroscopy; Khadijeh Rajabi; Elizabeth Gillis; Travis Fridgen; Memorial University of NL, St. John's, NF	4.43 pm	Research Award Presentation of the Waters Corp. Research Award
TOF pm 3:30	Gas Phase Hydration of Trapped Peptides:		
r	Kinetics; Xiangguo Shi; Joel H. Parks; Rowland	4:55 pm	Recipient of the Biemann Medal
	Institute at Harvard, Cambridge, MA		
TOF pm 3:50	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA	EMERGI	- 10:30 AM, WEDNESDAY MORNING NG MS TECHNIQUES FOR DRUGS AND TABOLITE IMAGING IN TISSUES Ballroom A
TOF pm 3:50	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the	EMERGI	NG MS TECHNIQUES FOR DRUGS AND TABOLITE IMAGING IN TISSUES Ballroom A
·	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the Dissociation Kinetics of Protein-Ligand	EMERGI ME	NG MS TECHNIQUES FOR DRUGS AND TABOLITE IMAGING IN TISSUES Ballroom A About Tissues, Compounds and Metabolites;
·	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the Dissociation Kinetics of Protein-Ligand Complexes in the Gas Phase; Elena Kitova; John	EMERGI ME	NG MS TECHNIQUES FOR DRUGS AND TABOLITE IMAGING IN TISSUES Ballroom A About Tissues, Compounds and Metabolites; Markus Stoeckli; Dieter Staab; Brendan Prideaux;
·	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the Dissociation Kinetics of Protein-Ligand Complexes in the Gas Phase; Elena Kitova; John Klassen; University of Alberta, Edmonton,	EMERGI ME	NG MS TECHNIQUES FOR DRUGS AND TABOLITE IMAGING IN TISSUES Ballroom A About Tissues, Compounds and Metabolites;
TOF pm 4:10	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the Dissociation Kinetics of Protein-Ligand Complexes in the Gas Phase; Elena Kitova; John Klassen; University of Alberta, Edmonton, Canada	WOA am 8:30	NG MS TECHNIQUES FOR DRUGS AND CTABOLITE IMAGING IN TISSUES Ballroom A About Tissues, Compounds and Metabolites; Markus Stoeckli; Dieter Staab; Brendan Prideaux; Novartis Institutes for BioMedical Research, Basel, Switzerland
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TOF pm 4:10 2:30 HDX FOI	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the Dissociation Kinetics of Protein-Ligand Complexes in the Gas Phase; Elena Kitova; John Klassen; University of Alberta, Edmonton, Canada 0-4:30 PM, TUESDAY AFTERNOON R PROTEIN STRUCTURE AND FOLDING Room 113 Structure of Lipid-Free and Lipid-Bound Human Apolipoprotein A-I by Hydrogen-Deuterium Exchange Analyzed by Mass Spectrometry; Palaniappan S Chetty ¹ ; Michael C Phillips ¹ ; Lund-Katz S ¹ ; Leland Mayne ¹ ; David	WOA am 8:30	NG MS TECHNIQUES FOR DRUGS AND CTABOLITE IMAGING IN TISSUES Ballroom A About Tissues, Compounds and Metabolites; Markus Stoeckli; Dieter Staab; Brendan Prideaux; Novartis Institutes for BioMedical Research, Basel, Switzerland Ambient Mass Spectrometric Imaging of Metabolites in Mus Musculus Brain and Arabidopsis Thaliana Leaf by Mid-Infrared Laser Ablation Electrospray Ionization; Peter Nemes¹; Ales Svatos²; Akos Vertes¹; ¹ George Washington University, Washington, DC; ² Max Planck Institute, Jena, Germany High-Field MALDI FTMS for Direct Pre- Clinical Imaging of Drug Distribution and
TOF pm 4:10 2:30 HDX FOI	Chirality: Effects on Folding and Aggregation of Peptides; Michael T. Bowers; Christian Bleiholder; Nicholas Dupuis; University of California, Santa Barbara, CA Influence of Configurational Entropy on the Dissociation Kinetics of Protein-Ligand Complexes in the Gas Phase; Elena Kitova; John Klassen; University of Alberta, Edmonton, Canada 1 — 4:30 PM, TUESDAY AFTERNOON R PROTEIN STRUCTURE AND FOLDING Room 113 Structure of Lipid-Free and Lipid-Bound Human Apolipoprotein A-I by Hydrogen-Deuterium Exchange Analyzed by Mass Spectrometry; Palaniappan S Chetty ¹ ; Michael C	WOA am 8:30 WOA am 8:50	NG MS TECHNIQUES FOR DRUGS AND CTABOLITE IMAGING IN TISSUES Ballroom A About Tissues, Compounds and Metabolites; Markus Stoeckli; Dieter Staab; Brendan Prideaux; Novartis Institutes for BioMedical Research, Basel, Switzerland Ambient Mass Spectrometric Imaging of Metabolites in Mus Musculus Brain and Arabidopsis Thaliana Leaf by Mid-Infrared Laser Ablation Electrospray Ionization; Peter Nemes¹; Ales Svatos²; Akos Vertes¹; ¹ George Washington University, Washington, DC; ² Max Planck Institute, Jena, Germany High-Field MALDI FTMS for Direct Pre- Clinical Imaging of Drug Distribution and Metabolism; Katherine A. Kellersberger¹; Michael L. Easterling¹; Santosh Kesari²; Claire
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Posttranslational Modifications on sRAGE

WUA am 9'50	Mass Spectrometric Imaging of Plant	WOC am 8:50	Phosphopeptide Characterization by
WOA am 9:50	Metabolites on Various Organs: Comparative	WOC um 0.50	Femtosecond Laser-Induced
	Study of Genetically Mutated Arabidopsis vs.		Ionization/Dissociation (fs-LID); Gavin E. Reid;
	Wild Type; Ji Hyun Jun ^{1,2} ; Zhenjiu Liu ^{1,2} ; Zhihong Song ^{2,3} ; Basil J. Nikolau ^{2,3} ; Edward S.		Christine L. Kalcic; Scott A. Smith; Marcos
	Yeung ^{1,2} ; Young Jin Lee ^{1,2} ; ¹ Department of		Dantus; Michigan State University, East Lansing, MI
	Chemistry, Iowa State University, Ames, IA;	WOC am 9:10	Ozone Induced Dissociation in Structure
	² Ames Lab, Ames, IA; ³ Department of		Elucidation; Huong Pham; Todd W Mitchell;
WO 4 10.10	Biochemistry, Iowa State University, Ames, IA		Michael Thomas; Stephen J Blanksby; University
WOA am 10:10	Spatial Querying of Mass Spectral Imaging Data Allows for Differential Analysis of	WOC am 9:30	of Wollongong, Wollongong, NSW, Australia Infrared Multiphoton Dissociation of Peptides
	Neurodegenerative Alterations in Tissue; Raf	WOC and 7.50	in a Dual Cell Linear Ion Trap Mass
	Van de Plas; Kristiaan Pelckmans; Thomas		Spectrometer ; Myles Gardner ¹ ; James Madsen ¹ ;
	Philips; Justin Vijay Louis; Bart De Moor;		Suncerae Smith ¹ ; Aaron Ledvina ² ; <u>Jennifer</u>
9.20	Etienne Waelkens; K.U.Leuven, Leuven, Belgium		Brodbelt ¹ ; ¹ University of Texas - Austin, Austin, TX; ² UW Madison, Madison, WI
	10:30 AM, WEDNESDAY MORNING DVANCES IN METABOLOMICS	WOC am 9:50	Homo- and Hetero-Oligomeric Complexes in
	Ballroom B		the Gas Phase Investigated by Ion Mobility and
WOB am 8:30	Metabolic Signatures of Human Drug		Tandem Mass Spectrometry; Elisabetta Boeri
	Response Phenotyping; Oliver Fiehn ¹ ; Gert		Erba; Brandon Ruotolo; Carol Robinson; University of Cambridge, Department of
	Wohlgemuth ¹ ; Dinesh Kumar Barupal ¹ ; Tobias Kind ¹ ; Rima Kaddurah-Daouk ² ; ¹ UC Davis,		Chemistry, Cambridge, UK
	Davis, CA; ² Duke University, Durham, NC	WOC am 10:10	Identification and Inhibition of Gas Phase
WOB am 8:50	UPLC-MS Metabolite Profiling to Investigate		Rearrangements of Protonated YAGFL
	the Influence of the Gut Microbiome on Host		Analogs and their Fragments; Ashley C.
	Metabolism; Elizabeth J Want ¹ ; Jonathan		<u>Gucinski</u> ; Asiri Galhena; Brittany R. Perkins; Arpad Somogyi, Vicki H. Wysocki, <i>University of</i>
	Swann ¹ ; Florian Geier ¹ ; James Sidaway ² ; Jeremy Nicholson ¹ ; Elaine Holmes ¹ ; Ian Wilson ² ;		Arizona, Tucson, AZ
	¹ imperial College, London, UK; ² Astra Zeneca,		10:30 AM, WEDNESDAY MORNING
	Macclesfield, UK	APPLICATION	ONS OF ION MOBILITY SPECTROMETRY
WOB am 9:10	Metabonomic Profiling and Metabolite Identification of Bromoethylamine, A Potent	WOD am 8:30	Room 204 Application Overview of Ion Mobility
	Nephrotoxicant; Petia Shipkova ¹ ; Serhiy	WOD alli 6.30	Spectrometry Coupled with Mass
	Hnatyshyn ¹ ; Mark Sanders ² ; Jeff Vassallo ¹ ;		Spectrometry; Herbert H. Hill; William F.
	Michael Reily ¹ ; Don Robertson ¹ ; Lois Lehman-		Siems; Kimberly A. Kaplan; Christina L.
	Mckeeman ¹ ; ¹ Bristol Myers Squibb, Princeton, NJ; ² Thermo Fisher Scientific, Somerset, NJ		Crawford; Eric J. Davis; Roberto Fernandez
WOB am 9:30	Identification and Quantification of		Maestre; Washington State University, Pullman, WA
	Metabolites in a Human Plasma Standard	WOD am 8:50	Ion Mobility Characterization of
	Reference Material by Multiple Mass		Carbohydrate:Protein Conformational
	Spectrometry Methods; Nathan G. Dodder; Ruth		Binding ; <u>Julie A. Leary</u> ¹ ; Raluca Stefanescu ² ;
	Dorole: Couthier Enne: Elizobeth A. MeCenze		
	Barak; Gauthier Eppe; Elizabeth A. McGaw; Stephen E. Stein: Karen W. Phinney: NIST.		Connie Jen ¹ ; ¹ UC Davis, Davis, CA; ² University
	Barak; Gauthier Eppe; Elizabeth A. McGaw; Stephen E. Stein; Karen W. Phinney; NIST, Gaithersburg, MD	WOD am 9:10	
WOB am 9:50	Stephen E. Stein; Karen W. Phinney; NIST, Gaithersburg, MD Accurate and Sensitive All-Ions Quantitation	WOD am 9:10	Connie Jen ¹ ; ¹ UC Davis, Davis, CA; ² University of Davis, Davis, CA A Shape Selective Study of Conformational Changes in Metal Containing Proteins; James
WOB am 9:50	Stephen E. Stein; Karen W. Phinney; NIST, Gaithersburg, MD Accurate and Sensitive All-Ions Quantitation Using a New Ultra High Resolution LCMS and	WOD am 9:10	Connie Jen ¹ ; ¹ UC Davis, Davis, CA; ² University of Davis, Davis, CA A Shape Selective Study of Conformational Changes in Metal Containing Proteins; James Scrivens ¹ ; Frances D L Kondrat ¹ ; Charlotte
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WOF am 9:30

Characterization of rf Plasma-Polymerized Compounds by MALDI Mass Spectrometry;

Lijuan Peng; Gary R. Kinsel; Southern Illinois National Laboratory, Richland, WA; ²Owlstone Ltd., Cambridge, UK University Carbondale, Carbondale, IL WOD am 10:10 WOF am 9:50 **Comparison of Electron Transfer Dissociation Observation of Neutral Molecule (Ion-Pair) Evaporation from Ionic Liquid Nanodroplets** and Collision-Induced Dissociation by Tandem Differential Mobility Analysis-Fragmentation of Multiply Charged Mass Spectrometry (DMA-MS); Christopher J. Polyethers; Tony Jackson¹; Gillian R. Hilton²; Hogan; Juan Fernandez de la Mora; Yale Susan E. Slade²; James Scrivens²; ¹AkzoNobel University - Mechanical Engineering, New CARG, Songjiang Industrial Estate, China; ²University of Warwick, Coventry, UK Haven, CT WOF am 10:10 Sample Spot Heterogeneity Investigated by 8:30 - 10:30 AM, WEDNESDAY MORNING MALDI - Imaging Mass Spectrometry; Steffen NEW DEVELOPMENTS IN BIOINFORMATICS M. Weidner; Jana Falkenhagen; Rolf-Dieter Exhibit Hall C Schulze; Andreas Thuenemann; WOE am 8:30 **A Fast Previewer for Shotgun Proteomics** Fed.Inst.f.Mat.Research, Berlin, Germany Data; Marshall W. Bern; Palo Alto Research 8:30 - 10:30 AM, WEDNESDAY MORNING Center, Palo Alto, CA COMPOSITIONAL ANALYSIS OF PETROLEUM BY MS WOE am 8:50 A Probabilistic Algorithm for Protein **Room 113** Identification Using a Simple, Realistic Model that Recognizes Degeneracy; Oliver Serang¹; WOG am 8:30 High Resolution MS/MS Techniques for the Jason Weston²; Michael J. Maccoss¹; William **Investigation of Crude Oils and its Fractions**; Noble¹; ¹*University of Washington, Seattle, WA*; Wolfgang Schrader¹; Saroj Panda¹; Kishore ²NEC Research, Princeton, NJ Sripada¹; Jan T. Andersson²; ¹Max-Planck Inst WOE am 9:10 **Spectral Profiles: A Novel Representation of** Coal Res., Mülheim / Ruhr, Germany; ²Inst. Tandem Mass Spectra and its Application for Inorg. and Analytical Chem. Univ. Muenster. Gapped Peptide Generation; Sangtae Kim; Muenster, Germany Nuno Bandeira; Pavel Pevzner; University of WOG am 8:50 Non-Invasive Molecular Characterization of California San Diego, La Jolla, CA Kerogen and its Insoluble Biopolymer WOE am 9:30 **Correlation of Database Entries and its Impact** Precursors by Fourier Transform Mass on Statistical Analysis in Peptide Spectrometry; Rachel L. Sleighter; Elodie Salmon; Heidi M. Bialk; Patrick G. Hatcher; Old Identification; Aleksey Y Ogurtsov; Gelio Alves; Yi-kuo Yu; National Center for Biotechnology Dominion University, Norfolk, VA Information, NLM, Bethesda, MD WOG am 9:10 **Comprehensive Characterization of Crude Oils** WOE am 9:50 Sequencing Proteins with MS/MS and a by Thermalanalysis Coupled to a Novel Photo-Homologous Reference Sequence; Xiaowen **Ionization Mass Spectrometer: Signatures of** Liu¹; Yonghua Han²; Denis Yuen³; <u>Bin Ma</u>¹; Vaporized Hydrocarbons and Asphaltene-**Pyrolysis**; Robert Geißler^{1,2}; Thorsten Streibel^{1,2}; ¹University of Waterloo, Waterloo, Canada; ²University of Western Ontario, London, ON; Mohammed Saraji^{1,2}; Ralf Zimmermann^{1,2}; ³Bioinformatics Solutions, Inc., Waterloo, ON ¹Universität Rostock, Rostock, Germany; ²Helmholtz Zentrum München, Oberschleissheim, WOE am 10:10 Proteogenomics of the Plague Bacterium, Yersinia Pestis; Sam Payne; Shih-Ting Huang; Germany Rembert Pieper; J Craig Venter Institute, WOG am 9:30 A Unified Theory of Asphaltene Structure; Amy Mckenna¹; Ryan P. Rodgers¹; Alan G. Rockville, MD Marshall³; ¹Natl High Magnetic Field Laboratory, 8:30 - 10:30 AM, WEDNESDAY MORNING Tallahassee, FL ²Ion Cyclotron Resonance Prog, MS OF POLYMERS/MATERIALS I: STRUCTURES AND Tallahassee, FL **PROPERTIES** WOG am 9:50 Fingerprinting Heteroatom Hydrocarbons Room 103 Using Ion Mobility – Mass Spectrometry: WOF am 8:30 Role of the Adducted Cation in the Release of Francisco Alberto Fernandez Lima; David H. Nitroxide End-Group of Controlled Synthetic Russell; Texas A&M University, College Station, Polymers in Mass Spectrometry; Michael Mazarin; Marion Girod; Stephane Viel; Trang WOG am 10:10 **High-energy Laser-induced Acoustic** Phan: Sylvain Marque: Stephane Humbel: **Desorption/Fourier Transform Ion Cyclotron** Laurence Charles; University Aix-Marseille I & Resonance Mass Spectrometric Analysis of III, Marseille Cedex 20, France Heavy Petroleum Products; David Pinkston; WOF am 8:50 **Inconsistencies in the Analysis of Large** Vanessa Gallardo; Steven Habicht; Hilkka Polycyclic Aromatic Hydrocarbons by Laser Kenttamaa; Purdue University, West Lafayette, IN **Desorption and Matrix Assisted Laser Desorption/Ionization Time-of-Flight Mass** 10:30 AM - 2:30 PM, WEDNESDAY Spectrometry; Hans Joachim Räder; Anna POSTER SESSION Cristadoro; Klaus Müllen; Max PLanck Institute for Polymer Research, Mainz, Germany **Exhibit Hall AB** WOF am 9:10 **Isotopically Labeled Nylon Provides Insight** into Oxidative and Hydrolytic Degradation Mechanisms; James Hochrein; Donald Bradley; Michael White; Steven Thornberg; Robert Bernstein; Sandia National Laboratories, Albuquerque, NM

37 ASMS Con	terence on Mass Spectrometry
2:30 -	4:30 PM, WEDNESDAY AFTERNOON
POL	YPEPTIDE ION FRAGMENTATION:
	THEORY AND EXPERIMENT
	Ballroom A
WOA pm 2:30	Enhancing ETD by Chemical Modifications
	that Increase Charge States of Peptides and
	Proteins; Brian L. Frey; April Jue; Aaron

- that Increase Charge States of Peptides and
 Proteins; Brian L. Frey; April Jue; Aaron
 Ledvina; Joshua J. Coon; Lloyd Smith; University
 of Wisconsin, Madison, WI
 WOA pm 2:50 Structural Motifs that Suppress Peptide Ion
- wOA pm 2:50

 Structural Motifs that Suppress Peptide Ion
 Fragmentation after Electron Capture; Takwah Dominic Chan; W. Y. Kelly Chan; The
 Chinese Univ. of Hong Kong, Hong Kong Sar,
 China
- WOA pm 3:10 Side-Chain Mediated Fragmentation of Peptide Radical Ions Produced in 157 nm Photodissociation; Liangyi Zhang; James P. Reilly; Indiana university, Bloomington, IN
- WOA pm 3:30 Effect of Chain Length on "b" Fragment
 Structures in Collision-Induced Cissociation of
 Protonated Peptides; Xian Chen¹; Long Yu¹; Jos
 Oomens²; Jeffrey Steill²; David H. Powell¹;
 Nicolas Polfer¹; ¹University of Florida,
 Gainesville, FL; ²FOM Rijnhuizen, Nieuwegein,
 Netherlands
- WOA pm 3:50 IRMPD and H/D Exchange Reveals that the HA b₂⁺ Ion Is a Mixture of Diketopiperazine and Oxazolone Structures; Brittany R. Perkins¹; Sung Hwan Yoon¹; Julia Chamot-rooke²; Arpad Somogyi¹; Vicki H. Wysocki¹; ¹The University of Arizona, Tucson, AZ; ²CNRS, Palaiseau, France
- WOA pm 4:10 DFT Modeling of Proton Transfer Reactions for the Formation of $(b_3)^+$ Ions within Alternative Amino Acid Model Tetrapeptides; Travis Cooper; Michael J. Van Stipdonk; Wichita State University, Wichita, KS

2:30 – 4:30 PM, WEDNESDAY AFTERNOON APPLICATION OF DIRECT/OPEN AIR IONIZATION TECHNIQUES FOR QUANTITATION OF DRUGS Ballroom B

- WOB pm 2:30 An Overview of Ambient Surface Sampling and Ionization Techniques; Gary J. Van Berkel; Oak Ridge National Laboratory, Oak Ridge, TN
- WOB pm 2:50 Quantitation of Drugs in Biological Matrices by Desorption Electrospray Ionization:
 Accuracy, Precision, Dynamic Range and Limit of Detection; Nicholas E. Manicke; Demian R. Ifa; R. Graham Cooks; Purdue University, West Lafayette, IN
- WOB pm 3:10 Eliminating Method Development, Sample Preparation and Chromatographic Separations in High-Throughput Bioanalysis Using DART on an Enhanced Resolution Triple-Quadrupole Mass Spectrometer; Elizabeth Crawford¹; Brian Musselman¹; Shaoxia Yu²; Jing-Tao Wu²;

 ¹IonSense, Inc., Saugus, MA; ²Millennium
- WOB pm 3:30

 Pharmaceuticals, Inc., Cambridge, MA

 Desorption Electrospray Ionization (DESI) for
 Direct Quantitation of Xenobiotics from Dried
 Blood Spots; Christopher A. Evans¹; Chester
 Bowen¹; Joseph H Kennedy²; Justin Wiseman³;

 GlaxoSmithKline, King of Prussia, PA;

 Prosolia, Inc, Indianapolis, IN; Prosolia, Inc.,
- WOB pm 3:50 Ambient Surface Sampling Mass Spectrometry Using a Fully Automated Chip-Based Nano-Electrospray System; Vilmos Kertesz; Gary J.

Indianapolis, IN

- Van Berkel; Oak Ridge National Laboratory, Oak Ridge, TN
- WOB pm 4:10 Application of Transmission Mode Desorption Electrospray Ionization (TM-DESI) to the Quantitative Analysis of Drugs; Joe Chipuk¹; Jennifer Brodbelt²; ¹University of Texas, Austin, TX; ²The University of Texas, Austin, TX

2:30 – 4:30 PM, WEDNESDAY AFTERNOON ADVANCES IN PROTEOGLYCAN AND CARBOHYDRATE ANALYSIS Room 201

- WOC pm 2:30 It's a Sweet World: Glycomic Analysis and Cellular Communication in the Extra- and Intracellular Space; Carol Nilsson¹; Huan He²; Mark R. Emmett³; Alan G. Marshall⁴; Roger A. Kroes⁶; Joseph R. Moskal⁶; Arugadoss Devakumar¹; Roslyn Dillon¹; Charles A. Conrad<SU; ¹Pfizer, Inc., San Diego, CA; ²Florida State University, Tallahassee, FL; ³Nat'l High Magnetic Field Lab, Tallahassee, FL; ⁴Ion Cyclotron Resonance Prog, Tallahassee, FL; ⁵M.D. Anderson Cancer Center
- WOC pm 2:50 New Perspectives on the Interpretation of Glycosaminoglycan Tandem Mass Spectra;
 Nancy Leymarie; Hicham Naimy; Gregory O
 Staples; Catherine E. Costello; Joseph Zaia; BU
 School of Medicine, Boston, MA
- WOC pm 3:10 Characterization of Heparin-Derived
 Oligosaccharides using Ion-Pair ReversedPhase LC/ESI-MS; Weibin Chen; Catalin
 Doneanu; John Gebler; Waters Corporation,
 Milford, MA
- WOC pm 3:30 Sequential Enrichment and Structural
 Analysis of Sulfated N-Glycans through AnionExchange Chromatography and MALDIMS/MS; Ming Lei; Yehia Mechref; Milos V.
 Novotny; Indiana university, Bloomington, IN
- WOC pm 3:50 Exploring the N-linked Glycome for Early
 Detection of Epithelial Ovarian Cancer by
 NanoLC FT-ICR Mass Spectrometry; Michael
 S. Bereman¹; William A. Cliby²; David C.
 Muddiman¹; ¹North Carolina State University,
 Raleigh, NC; ²Mayo Clinic, Rochester, MN
- WOC pm 4:10 The Development of Methods towards High Throughput Clinical Glycomics; Scott R.

 Kronewitter¹; Kyle S. Peacock¹; Maria Lorna de Leoz¹; Hyun Joo An¹; Suzanne Miyamoto²; Gary S. Leiserowitz²; Helen K. Chew²; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA; ²UC Davis Cancer Center, Davis, CA

2:30 – 4:30 PM, WEDNESDAY AFTERNOON DEVELOPMENTS IN IMAGING INSTRUMENTATION Room 204

- WOD pm 2:30 New Strategies for Imaging Mass Spectrometry Using C60-SIMS and MALDI Probes; Anthony Carado¹; Melissa Passarelli¹; Julie Wingate²; Alexandre Loboda²; Nick Winograd¹; ¹Penn State University, University Park, PA; ²MDS Analytical Technologies, Concord, ON
- WOD pm 2:50 High Resolution C-60 SIMS and MALDI
 Microscopy Using a Delay Line Detector;
 Leendert A. Klerk¹; Andriy Kharchenko¹; Luke
 Macaleese¹; Nicholas P. Lockyer²; John
 Vickerman²; Ron M.A. Heeren¹; ¹FOM Institute
 for Atomic and Molecular Physics, Amsterdam,
 Netherlands; ²University of Manchester,
 Manchester, UK

N-Nitrosodiphenylamine Formation during

2			<u> </u>
WOD pm 3:10	Digital Imaging Mass Spectrometry with the TimePix; Casimir Bamberger ¹ ; Andreas Bamberger ² ; ¹ Scripps Research Institute, La Jolla, CA; ² Physics Institute, Albert-Ludwigs University,	2:30 – 4:30 PM, WEDNESDAY AFTERNOON MS OF POLYMERS/MATERIALS II: HPLC AND ION MOBILITY SEPARATION Room 103	
	Freiburg i. Br., Germany	WOF pm 2:30	Polymer Analysis Using GPC, Thermospray
WOD pm 3:30	Investigation of Nanoscale Chemical Imaging	WOT pill 2.30	Deposition and MALDI-TOF Mass
	via Tip-Enhanced, Near-Field		
	Desorption/Ionization Mass Spectrometry at		Spectrometry; Mark Arnould; Xerox, Webster,
	Atmospheric Pressure; James A. Bradshaw;	WOE 2.50	NY Standard Changetonication of a Complex
	Kent A Meyer; Olga S. Ovchinnikova; Douglas E.	WOF pm 2:50	Structural Characterization of a Complex
	Goeringer; Oak Ridge National Laboratory, Oak		Nonionic Surfactant by LC-MS ⁿ ; Nilufer Solak;
	Ridge, TN		Chrys Wesdemiotis; <i>The University of Akron</i> ,
WOD pm 3:50	Laser Induced Material Transfer Combined	WOE 2.10	Akron, OH
,, ob p 5.5 v	with MALDI MS for a Sub-cellular Imaging;	WOF pm 3:10	Characterization on Poly (n-Butyl Acrylate)s
	Andrey I. Zavalin; Peggi Angel; Richard M.		by LC/ESI-MS ⁿ ; <u>Junkan Song</u> ¹ ; Jan W. van Velde ¹ ; Luc L.T. Vertommen ¹ ; Ron M.A.
	Caprioli; Vanderbilt Univ Sch of Med, Nashville,		Heeren ² ; Oscar F. van den Brink ¹ ; ¹ Research,
	TN		Development and Innovation, AkzoNobel,
WOD pm 4:10	MALDI-Tissue Imaging at High Resolution		Arnhem, The Netherlands; ² FOM Inst.
1	and Speed: Essential Steps Towards its		Atomic/Molecular Phy, Amsterdam, The
	Applications in Histology; Soeren-Oliver		Netherlands
	Deininger; <u>Detlev Suckau</u> ; Michael Becker; M.	WOF pm 3:30	Recent Mass Spectrometric Developments and
	Schuerenberg; Bruker Daltonik GmbH, Bremen,	WO1 piii 3.30	Investigations for Age Determination of Ball
	Germany		Point Ink Entries on Paper; Dieter Kirsch ¹ ;
2:30 -	4:30 PM, WEDNESDAY AFTERNOON		Vincent Guillou ¹ ; Bernhard Spengler ² ; Peter
	TERIZATION OF MEMBRANE PROTEINS		Seiler ¹ ; Fritz Koehler ¹ ; ¹ Bundeskriminalamt,
	Exhibit Hall C		Wiesbaden, Germany; ² Analytical Chemistry,
WOE pm 2:30	Filter Aided Sample Preparation (FASP)		Giessen, Germany
	Combines the Advantages of In-Gel and In-	WOF pm 3:50	Identification of Poly(p-phenylene
	Solution Digestion; Jacek R. Wisniewski;		terephthalamide) Branching and Metathesis
	Nagarjuna Nagaraj; Alexandre Zougman;		Products ; Anthony P. Gies; David M. Hercules;
	Matthias Mann; Max-Planck-Institute of		Vanderbilt University, Nashville, TN
*****	Biochemistry, D-82152 Martinsried, Germany	WOF pm 4:10	Ion Mobility Spectrometry-Mass Spectrometry
WOE pm 2:50	Quantitative Assessment of Enhanced		of Star-Branched Poly(ethylene glycols);
	Recovery of Hydrophobic Peptides from		Barbara S. Larsen ² ; Calvin A. Austin ¹ ; Brian
	Reversed Phase Chromatography at Elevated		Bohrer ³ ; Ellen D. Inutan ¹ ; Sadish Karunaweera ¹ ;
	Temperatures; Kelli G. Kline; Sarah M. Moore;		David E. Clemmer ³ ; Sarah Trimpin ¹ ; ¹ Wayne State University, Detroit, MI; ² The DuPont
	Christine C. Wu; <i>University of Colorado School of Medicine, Aurora, CO</i>		Company, Wilmington, DE; ³ Indiana University,
WOE pm 3:10	Scoring Peptides by their Retention Time: A		Bloomington, IN
11 OL pin 3.10	Method that both Predicts and Incorporates	2:30 -	4:30 PM, WEDNESDAY AFTERNOON
	Retention Time into a Peptide-Spectrum		ND EMERGING ENVIRONMENTAL
	Match Scoring Function; Lukas Käll ¹ ; Michael	1,157	CONTAMINANTS
	J. Maccoss ² ; William Noble ² ; ¹ Stockholm		Room 113
	University, Stockholm, Sweden; ² University of	WOG pm 2:30	Emerging Environmental Contaminants:
	Washington, Seattle, WA		What's New; Susan Richardson; US EPA,
WOE pm 3:30	Strategies for MALDI Imaging Mass		Athens, GA
	Spectrometry of Integral Membrane Proteins;	WOG pm 2:50	Analysis of Illicit Drugs and Metabolites in
	Angus C. Grey ¹ ; Pierre Chaurand ¹ ; Richard M.		Wastewater Derived from an Educational
	Caprioli ² ; Kevin L. Schey ¹ ; ¹ Vanderbilt University, Nashville, TN; ² Vanderbilt Univ Sch		Institution ; M. Paul Chiarelli ¹ ; Sara Castiglioni ² ;
	Oniversity, Nashville, TN; Vanaerbiit Univ Sch of Med, Nashville, TN		Deepika Panawennage ¹ ; Ettore Zuccato ² ; Enrico
WOE pm 3:50	The Subunits of a Large Integral Membrane		Davoli ² ; ¹ Loyola University, Chicago, IL; ² Mario
WOL pili 3.30	Protein Complex characterized by Top-Down	W00 210	Negri Institute, Milano, Italy
	Fourier-Transform Mass Spectrometry; Julian	WOG pm 3:10	Liquid Chromatography Accurate Mass
	Whitelegge ¹ ; Christopher Ryan ¹ ; Puneet Souda ¹ ;		Spectrometry Screening Analysis of
	Sara Bassilian ¹ ; Kym Faull ¹ ; Balakumar		Pharmaceuticals in Fish Collected from Effluent-Dominated Streams, Alejandro J.
	Thangaraj ² ; Petra Fromme ² ; ¹ University of		Ramirez ¹ ; C. Kevin Chambliss ^{1,3} ; Bryan W.
	California LA, Los Angeles, CA; ² Arizona State		Brooks ² ; ¹ Mass Spectrometry Core Facility,
	University, Tempe, AZ		Baylor University, Waco, TX; ² Environmental
WOE pm 4:10	Mass Spectrometry of Integral Membrane		Studies, Baylor University, Waco, TX; ³ Chemistry
	Transporters from Detergent Micelles Reveals		and Biochemistry, Baylor University, Waco, TX
	their Stoichiometry and Interactions;	WOG pm 3:30	Fast Analysis of Pharmaceuticals in Water
	Shoshanna C. Isaacson; Nelson P. Barrera; Min	•	following EPA Method 1694: Applications of
	Zhou; Dijana Matak-Vinkovic; Carol V.		UHPLC-MS/MS; Michael Thurman; Imma
	Robinson; <i>University of Cambridge, Cambridge, UK</i>	****	Ferrer; University of Colorado, Boulder, CO
	ON	WOG pm 3:50	LC/MS/MS Characterization of Mechanisms of

Water Chloramination Disinfection; Wenjun Zhou^{1,1}; Jessica Boyd^{1,2}; Feng Qin^{1,2}; Yuli Zhao^{1,2}; Xing-fang Li^{1,2}; ¹, Edmonton, Canada; ²University of Alberta, Edmonton, AB WOG pm 4:10 A Novel Technique Utilizing SBSE and DART-TOF for the Analysis of Pharmaceutical and Pesticide Contaminants in Aqueous Media; Kathleen Brooks Loftin¹; <u>Timothy P. Griffin</u>¹; Christian A. Clausen III²; Robert B. Cody³; A. John Dane³; ¹NASA- Kennedy Space Center, Kennedy Space Center, FL; ²University of Central Florida, Orlando, FL; ³JEOL USA, Inc., Peabody, ThOB am 9:30 4:45 - 5:30 PM, WEDNESDAY ASMS MEETING Wine and Beer, Prizes and More!! Exhibit Hall C 8:30-10:30, THURSDAY MORNING MS OF PEPTIDE AND PROTEIN DRUGS Ballroom A ThOB am 9:50 ThOA am 8:30 Application of Immunoglobulin Degrading Enzyme IdeS and LC-MS Analysis as Powerful **Characterization Method for Therapeutic** Antibodies; Anne Zeck; Joerg Regula; Wilma Dormeyer; Georg Drabner; Hans Rainer Völger; Hans Koll; Roche Diagnostics GmbH, Penzberg, Germany ThOA am 8:50 Stability of Protein Therapeutics under Near-Physiological Conditions: Conformation and Dynamics of Acid-β-Glucosidase; Cedric Bobst¹; John J. Thomas²; Paul Salinas²; Rinat Abzalimov¹; Philip J. Savickas²; Igor A. Kaltashov¹; ¹University of Massachusetts, ThOC am 8:30 Amherst, MA; ²Shire HGT, Cambridge, MA ThOA am 9:10 Application of Fast Liquid Chromatography-UHR Time-of-Flight Mass Spectrometry to the **Characterization of Pharmaceutical Grade** rBet v 1 Birch Pollen Allergen; Emmanuel Nony; Emmanuel Godat; Pierrick Lemoine; ThOC am 8:50 Thierry Batard; Philippe Moingeon; Stallergenes, Antony, France ThOA am 9:30 The Development of a Method for the **Determination of a Proprietary Domain** Antibody Therapeutic Using UPLC-MS/MS; ThOC am 9:10 Matthew Szapacs; Jonathan Kehler; Sharon Boram; David Citerone; GlaxoSmithKline, Blue Bell . PA ThOA am 9:50 Sequence Elucidation of Unknown Peptide of High Doping Potential by Electrospray **Ionization Mass Spectrometry**; Fuyu Guan¹; ThOC am 9:30 Cornelius Uboh²; Lawrence R. Soma¹; Jeffrey Rudy², ¹University of Pennsylvania, West Chester, PA; ²PA Equine Toxicology, West Chester, PA ThOA am 10:10 The Challenging Topography of the LC/MS Peptide Map; Scott Berger; Asish Chakraborty; Weibin Chen; Waters Corporation, Milford, MA 8:30-10:30, THURSDAY MORNING NOVEL LC-MS TECHNIQUES FOR REGULATED **BIOANALYSIS OF DRUGS** Ballroom B

ThOB am 8:30 HPLC-APPI-MS/MS Used as a Quantification Tool for Plasma Levels Studies of Cholecalciferol, Cinobufagin and Bisphenol-A; Julien Breault-Turcot¹; Jean-Francois Levesque²; Sebastien Gagne²; ¹Université de Montréal,

Montréal, QC; ²Merck Frosst Canada & Co, Kirkland, Canada

ThOB am 8:50 Is the Quantum Vantage Triple Quadrupole

Mass Spectrometer Suitable for Regulated
Bioanalysis? Jim Shen; Roger N. Hayes; Jennifer
N. Cunliffe; Schering-Plough Research Institute,
Summit, NJ

ThOB am 9:10 Combining High Speed Chromatography and Multistream HPLC Systems to Increase Productivity and Efficiency in the Bioanalytical Laboratory; John Gibbons¹; Chad Briscoe²; Min J. Yang¹; Adrian Taylor¹; David Cox¹; ¹MDS Analytical Technologies, Concord, Canada; ²MDS Pharma Services, Lincoln, NE

ChOB am 9:30 Quantification of Endogenous Leptin and Recombinant-Methionyl Human Leptin in Clinical Plasma Samples at Low-Nanomolar Levels by Immunocapture / Mass Spectrometry; Yan Wang; Chris Bellows; Kristine de Dios; Swati Gupta; Joseph S. Heilig; Steven Taylor; Amylin Pharmaceuticals, Inc., San Diego, CA

hOB am 9:50 Monitoring Age Related Changes of
Metabolism of Doxorubicin Using HPLC-LIFMS/MS; Joseph B Katzenmeyer; Yaohua Wang;
Edgar A. Arriaga; University of Minnesota,
Minneapolis, MN

ThOB am 10:10 Analysis of Drug Residues in Milk by On-Line SPE/LC/MS/MS; Claude Mallet; Claude Mallet; Waters Corporation, Milford, MA

8:30-10:30, THURSDAY MORNING MASS SPECTROMETRY AT THE INTERFACE BETWEEN CHEMISTRY AND BIOLOGY Room 201

Chemical Biology Approaches to
Understanding the Regulation of Nuclear
Receptors; Michael J. Chalmers; Scott A. Busby;
Ruben Garcia-Ordonez; Monica Istrate; Naresh
Kumar; Scott Novick; Bruce D. Pascal; Jun
Zhang; Patrick R. Griffin; The Scripps Research
Institute, Jupiter, FL

hOC am 8:50 Probing Drug Mechanism of Action via
Cellular Metabolomics: Thymineless Death
and Glycineless Stasis; Yun Kyung (Sophia)
Kwon; Joshua Rabinowitz; Princeton University,
Princeton NI

Identification of Native Divalent and Trivalent
Cross-linked Amino Acids from Left
Ventricular Cardiac Collagen; Forrest S.E.
Helfrich; Timothy J. Black; Eric D. Dodds; Qianli
Yu; Doug F. Larson; Vicki H. Wysocki;
University of Arizona, Tucson, AZ

OC am 9:30 FAC-MS Uncovers New Effectors for Old
Transcriptional Regulators, Discovery of Novel
Transcription Factor Effectors for MetJ;
Ricardo Marti-arbona²; Hiro Teshima³; Penny
Anderson¹; Pat J. Unkefer⁴; Clifford Unkefer¹;

¹Los Alamos National Laboratory, Los Alamos,
NM; ²Los Alamos National Laborato, Los
Alamos, NM; ³Los Alamos National Lab., Los
Alamos, NM; ⁴Los Alamos National Lab, Los

ThOC am 9:50 Substantially Improved Reproducibility and Precision in Quantitative Proteomics Assays by Targeted Data Acquisition; Frank Fischer; Mikhail Savitski; Gavain Sweetman; Marcus Bantscheff; Cellzome AG, Heidelberg, Germany

Alamos, NM

ThOC am 10:10 Characterizing the Partitioning between RNA
Regulatory Structures in the Moloney Murine
Leukemia Virus Using Antisense LNAs; Arie
Hawkins; Daniele Fabris; U. Maryland Baltimore
County, Baltimore, MD

8:30-10:30, THURSDAY MORNING FUNDAMENTAL ASPECTS OF ION/ELECTRON AND ION/ION REACTIONS Room 204

ThOD am 8:30 When Positive and Negative Ions Meet:

Energetics, Structure, Mechanisms and More!

Evan R. Williams; William A. Donald; Ryan D.

Leib; James S. Prell; University of California,

Berkeley, CA

ThOD am 8:50 Electron-Induced Rearrangements in Histidine and Arginine Peptides; Frantisek Turecek¹; Jean Wyer²; Annelie Ehlerding²; Henning Zettergren²; Preben Hvelplund²; Steen Brondsted Nielsen²; Benjamin Bythell³; Bela Paizs³; ¹University of Washington, Seattle, WA; ²University of Aarhus, Aarhus, Denmark; ³German Cancer Research Institute, Heidelberg, Germany

ThOD am 9:10 Uncommon Radical Rearrangements in

Electron Capture Dissociation of Peptide Ions;

Cheng Lin¹; Xiaojuan Li¹; Nadezda P. Sargaeva¹;

Peter B. O'connor²; ¹Boston University School of

Medicine, Boston, MA; ²University of Warwick,

Coventry, UK

ThOD am 9:30 Peptide Conformation Selectivity in Electron
Capture and Transfer Dissociation; Yury O.
Tsybin; Hisham Ben Hamidane; Aleksey
Vorobyev; Matthew Wodrich; Clemence
Corminboeuf; Ecole Polytechnique Federale,
Lausanne, Switzerland

ThOD am 9:50 Mechanisms of Resonance Electron Capture by
Neutral Peptides. Parallel with the ECD/ETD
Mechanisms; Yury V. Vasil'ey; Douglas F.
Barofsky; Max L. Deinzer; Oregon State
University, Corvallis, OR

ThOD am 10:10 Reverse Electron Transfer Dissociation on Anionic Peptides Using Molecular Radical Cations; Nicolas Polfer¹; Malwina Huzarska¹; Desmond Kaplan²; Michael Easterling²;

¹University of Florida, Gainesville, FL; ²Bruker Daltonics, inc., Billerica, MA

8:30-10:30, THURSDAY MORNING ADVANCES IN GLOBAL PHOSPHOPROTEIN Exhibit Hall C

ThOE am 8:30 Biological Insights from Quantitative Analysis of Phosphorylation-Mediated Signaling Networks; Forest M White; MIT, Cambridge, MA

ThOE am 8:50 Why Large-Scale Phosphoproteomic Analyses
Benefit from the Joint Use of Collision and
Electron-Based Fragmentation Methods; Paul
A. Grimsrud; Danielle L. Swaney; Craig D.
Wenger; Desiree den Os; Michael R. Sussman;
Jean-Michel M. Ane; Joshua J. Coon; University
of Wisconsin, Madison, WI

ThOE am 9:10 Large-Scale Proteomic Analyses Reveal that
Aurora B is a Master Kinase Regulating the Cphase Cytoskeleton; Nurhan Ozlu³; Flavio
Monigatti³; Bernhard Renard²; Christine Field¹;
Hanno Steen³; Timothy Mitchison¹; Judith Steen³;

¹Harvard Medical School, Boston, MA;

²University of Heidelberg, Heidelberg, Germany;

³Harvard Medical School/Children's Hospital Boston, Boston, MA

ThOE am 9:30

Tyrosine Phosphorylation Signaling Network Analysis Reveals That Focal Adhesion Kinase is Important during Mouse Embryonic Stem Cell Differentiation; Yu Lu¹; Scott Ficarro²; Yi Zhang²; Manor Askenazi³; Jignesh Parikh²; Shaojuan Li²; C. John Luckey⁴; Jarrod Marto¹; ¹Dana-Farber Cancer Institute, Harvard Medical Scho, Boston, MA; ²Dana-Farber Cancer Institute, Boston, MA; ³Dana-Farber Cancer Institute and Hebrew University, Boston, MA; ⁴Brigham Women's Hospital, Boston, MA

ThOE am 9:50 Analysis by Microfluidic LC-MS/MS with Integrated Phosphopeptide Enrichment Reveals Dynamic Human Milk Protein Phosphorylation during Lactation; John W.

Froehlich¹; Ning Tang²; Keith Waddell²; Karsten Kraiczek²; Martin Vollmer²; Tom Van De Goor²; Rudolf Grimm²; Carlito B. Lebrilla¹; ¹University of California, Davis, CA; ²Agilent Technologies, Santa Clara, CA

ThOE am 10:10 In Vitro and In Vivo Study of Phosphorylated
Histidine Containing Peptides by NanoESI/nano-HPLC Tandem Mass Spectrometry;
Bryan M. Ham¹; Feng Yang²; Samuel O.
Purvine²; Rui Zhao²; Richard D. Smith²; Mary S.
Lipton²; ¹Customs & Border Protection, Newark,
NJ; ²Pacific Northwest National Laboratory,
Richland, WA

8:30-10:30, THURSDAY MORNING NUCLEIC ACID MS Room 103

ThOF am 8:30 Probing the Effects of Sodium Cationization on the Structure and Stability of Nucleic Acids via IRMPD Action Spectroscopy and Theory;

Mary T. Rodgers¹; B. Scott Fales¹; Nathaniel O. Fujamade¹; Nuwan Hallowita¹; Yuan-wei Nei¹;

Jos Oomens²; Jeffrey Steill²; ¹Wayne State
University, Detroit, MI; ²FOM Rijnhuizen,
Nieuwegein, Netherlands

ThOF am 8:50 IR Spectroscopy of DNA Single Strands,
Duplexes and I-Motif to Characterize their Gas
Phase Structure; Frederic Rosu¹; Valerie
Gabelica¹; Gilles Gregoire²; Charles Desfrancois²;
Jean-Pierre Schermann²; Joel Lemaire³; Edwin De
Pauw⁴; ¹University of Liege, Liege, Belgium;
²UMR 7538 CNRS, Université Paris 13, Paris,
France; ³Laboratoire de Chimie Physique, Orsay,
France; ⁴Liege University, Liege, Belgium

ThOF am 9:30 Determining RNA Modifications Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS); Stefan Weidt¹; Angus Lamond²; Pat Langridge-smith¹; C. Logan Mackay¹; ¹University of Edinburgh, Edinburgh, UK; ²University of Dundee, Dundee, UK

ThOF am 9:30 Investigating Higher-Order Structure of
Nucleic Acids by IRMPD in FTICR Mass
Spectrometry; Joshua Wilhide; Katherine
Kellersberger; Daniele Fabris; U. Maryland
Baltimore County, Baltimore, MD

ThOF am 9:50 LC-MS/MS for Assessing the Formation and the Cytotoxic/Mutagenic Properties of the Thymidine Glycol/8-Oxo-2'-Deoxyguanosine Tandem Lesion; Yong Jiang; Bifeng Yuan; Yuesong Wang; Yinsheng Wang; University of California, Riverside, CA

ThOF am 10:10 Identifying LEF1 IRES Protein Complexes by
Mass Spectrometry; Becky Tsai; Xiaorong
Wang; Lan Huang; Marian Waterman; University
of California, Irvine, CA

8:30-10:30, THURSDAY MORNING AEROSOL MS Room 113

ThOG am 8:30 What Aerosol Mass Spectrometers Tell Us about the Air We Breathe; Murray V. Johnston; University of Delaware, Newark, DE

ThOG am 8:50 Detection of Aerosol Particles with a Quadrupole Ion Trap Mass Spectrometer; G. Asher Newsome; Elias P. Rosen; Richard M. Kamens; Tomas Baer; Gary L. Glish; University of North Carolina, Chapel Hill, NC

ThOG am 9:10 Reactive Uptake of Trimethylamine into Ammonium Nitrate Particles Using an IT-TOF Aerosol Mass Spectrometer; Julie A. Lloyd¹; Katherine J. Heaton²; Murray V. Johnston³;

¹University of the Sciences in Philadelphia, Philadelphia, PA; ²Phoenix S&T, Chester, PA;

³University of Delaware, Newark, DE

ThOG am 9:30 Two-Step Laser Ionization TOF-Mass
Spectrometry for Analysis of Intact Organic
Molecules from Individual Aerosol Particles:
Detection of Organic Aerosol-Source Tracers;
Matthias Bente²; Martin Sklortz¹; Thorsten
Streibel^{1,2}; Ralf Zimmermann^{1,2}; ¹Universität
Rostock, Rostock, Germany; ²Helmholtz Zentrum
München, Oberschleissheim, Germany

ThOG am 9:50 Nanoparticle Atomic Composition from NAMS Spectra; Christopher A. Zordan; Murray V. Johnston; University of Delaware, Newark, DE

ThOG am 10:10 Miniaturized MS-based System for Rapid Detection and Identification of Chemical and Biological Warfare Agents and Toxic Industrial Chemicals; Berk Oktem; Vadym D. Berkout; Andrey N. Vilkov; Thomas D. Saul; Appavu K. Sundaram; Seshu K. Gudlavalleti; Jane Razumovski; Chaminda M. Gamage; Eugene Moskovets; Robert M. Serino; Vladimir M. Doroshenko; Science and Engineering Serv. Inc., Columbia, MD

10:30 AM – 2:30 PM, THURSDAY POSTER SESSION Exhibit Hall AB

2:30-4:30, THURSDAY AFTERNOON IMAGING APPLICATIONS WITH MS Ballroom A

ThOA pm 2:30 Capturing Complex Multi-Natural Product
Discussions between Bacteria; Pieter Dorrestein;
University of California, San Diego, Skaggs
school, La Jolla, CA

ThOA pm 2:50

Tissue Preparation for the in situ MALDI MS
Imaging of Proteins, Lipids, and Small
Molecules at Cellular Resolution; Nathalie Y.
R. Agar²; Paul J. Kowalski³; John H. Wong¹;
Kristin J. Boggio¹; Rebecca M. Lazarus¹; Jeffrey
N. Agar¹; ¹Brandeis University, Chemistry,
Waltham, MA; ²Harvard Medical School,
Neurosurgery, Boston, MA; ³Bruker Daltonics,
Inc., Billerica, MA

ThOA pm 3:10 Total Solvent-Free Analysis Using Mass Spectrometry; Sarah Trimpin¹; Calvin Austin¹; Charles N. Mcewen²; Michael Walker³; ¹Wayne State University, Detroit, MI; ²Univ. of the Sciences in PA, Philadelphia, PA; ³Indiana University, Bloomington, IN

ThOA pm 3:30 Novel "Tomography" Mass Spectrometry
Tissue Imaging Method; Corina Mayrhofer¹;
Alexander R. Zubarev¹; Eva Fung¹; Roman A.
Zubarev²; ¹Uppsala University, Uppsala,
Sweden; ²Karolinska Institute, Stockholm,
SWEDEN

ThOA pm 3:50 Tissue-less Tissue Imaging: Molecular Printing
Using Affinity-Enhanced Chromatographic
Surfaces for MALDI TOF/TOF; Mariana Rusa;
Steve Roth; Matthew Hammond; Vanitha
Thulasiraman; Enrique Dalmasso; Fiona Plows;
Bio-Rad Laboratories, Inc., Hercules, CA

ThOA pm 4:10 Tissue Imaging of Neuropeptides by MALDI
Orbitrap MS; Peter D. Verhaert¹; Martijn
Pinkse¹; Maria C. Prieto Conaway²; **IDelft
University of Technology, Delft, Netherlands;
Thermo Fisher Scientific, San Jose, CA

2:30-4:30, THURSDAY AFTERNOON ADME ANALYSIS BY LASER DESORPTION AND OTHER NEW MS TECHNIQUES Ballroom B

ThOB pm 2:30 **Utility of MALDI-MS for ADME Studies**; Walter Korfmacher; *Schering-Plough, Kenilworth*, *NJ*

ThOB pm 2:50 Validation and Application of a Method for Quantification of Antidepressants in Plasma Samples Using a MALDI-QqQ system; Timothy Sangster¹; Siew Mun Wan¹; Robert Macneill¹; Daniel Lebre²; Pauline J. Vollmerhaus²; Gary Impey²; ¹HLS, East Millstone, NJ; ²Applied Biosystems/MDS Analytical Technologies, Concord. ON. Canada

ThOB pm 3:10 Investigation of Individual Drug and Metabolite Whole-Body Distributions via Accurate Mass Imaging MALDI Mass Spectrometry; Sheerin Khatib-Shahidi¹; Sucharita Dutta²; Yingying Huang²; Caroline Ding²; Maria C. Prieto Conaway²; Cornelis Hop¹; Patrick J. Rudewicz¹; ¹ Genentech, Inc., South San Francisco, CA; ² Thermo Fisher Scientific, San Jose, CA

ThOB pm 3:30 High Throughput Profiling of Drug
Metabolites Using Low Pressure LC/Orbitrap
MS: An Alternative Approach to UPLC/MS;
Qian Ruan; Li Ma; Yuan-qing Xia; Mohammed
Jemal; William Humphreys; Mingshe Zhu;
Bristol-Myers Squibb, Princeton, NJ

ThOB pm 3:50 Combined Multiple Survey Approach for Sulfate Metabolite Identification Studies Using a Hybrid Linear Ion Trap Triple Quadrupole Mass Analyzer; Shaokun Pang¹; Loren Olson²; Elliott Jones²; Rongda Xu¹; Daniel B. Kassel¹; ¹Takeda San Diego, Inc., San Diego, CA; ²Applied Biosystems, San Jose, CA

ThOB pm 4:10 Analysis of *in-vivo* Samples for Metabolite Identification with a Prototype QTof Mass Spectrometer with Enhanced Dynamic Range and Spectral Resolution; Jose Castro-perez¹; Kate Yu¹; John P. Shockcor¹; Henry Y. Shion¹; Emma Marsden-edwards²; Jason L Wildgoose²; Martin Green²; John B Hoyes²; Alistair Wal; ¹Waters Corporation, Milford, MA; ²waters, Manchester, UK; ³Showa University, Tokyo, Japan

2:30-4:30, THURSDAY AFTERNOON NEW DEVELOPMENTS IN IONIZATION Room 201

ThOC pm 2:30 Separations in a Single Droplet: Understanding Surface Effects in Electrospray Ionization;

Kaveh Jorabchi; Lloyd Smith; University of Wisconsin, Madison, WI

ThOC pm 2:50 Charge-State Reduction of Synthetic Polymers by SEC-ESI-MS with Postcolumn Addition of Ionic Surfactants; Andreas Nasioudis¹; William F. Joyce²; Jan W. van Velde¹; Oscar F. van den Brink¹; ¹AkzoNobel Research, Development & Innovation, Arnhem, Netherlands; ²AkzoNobel Surface Chemistry LLC, Brewster, NY

ThOC pm 3:10 New Reagents for ESI "Supercharging" of Noncovalent Protein Complexes and Denatured Proteins; Rachel O. Loo; Shirley Lomeli; Sheng Yin; Joseph A. Loo; UCLA, Los Angeles, CA

ThOC pm 3:30 A Simple Method for the Determination of Electrospray Response Factors of Non-Covalent Complexes: Application to DNA G-Quadruplex Binding and Self-Assembly;

Valerie Gabelica¹; Jussara Amato²; Giorgia
Oliviero²; Frederic Rosu¹; Edwin De Pauw¹;

¹University of Liege, Liège, Belgium; ²University Federico II, Napoli, Italy

ThOC pm 3:50 AC Electrospray: A New Soft Ionization
Technique for Mass Spectrometry; Nishant
Chetwani; David Go; Hsueh-Chia Chang;
University of Notre Dame, Notre Dame, IN

ThOC pm 4:10

Positron Ionization Mass Spectrometry of
Biomolecules; Panagiotis G Papoulias¹; Alan
Sebastian⁴; Eugene Surdutovich³; Kristina
Hakansson²; Walter E Kauppila⁴; Philip
Andrews²; ¹National Resource For Proteo, Ann
Arbor, MI; ²University of Michigan, Ann Arbor,
MI; ³Oakland University, Rochester, MI; ⁴Wayne
State University, Detroit, MI

2:30-4:30, THURSDAY AFTERNOON ETD/ECD/EDD APPLICATIONS Room 204

ThOD pm 2:30 Ion/Ion and Ion/Electron Dissociation

Methods: Characteristics and Instrumentation;

John E. P. Syka¹; James L. Stephenson²; ¹Thermo

Fisher Scientific, Charlottesville, VA; ²Research

Triangle Institute, Research Triangle Park, NC

ThOD pm 2:50 Reverse Electron Transfer Dissociation (rETD) of Glycosaminoglycan Negative Ions; Jeremy Wolff²; Franklin E. Leach III¹; Tatiana Laremore³; Robert J. Linhardt³; Desmond Kaplan²; Michael Easterling²; Jon Amster¹;

¹University of Georgia, Athens, GA; ²Bruker Daltonics, Billerica, MA; ³Rensselaer Polytechnic Institute, Troy, NY

ThOD pm 3:10 ETD and the Combinatorial Epigenetic
Histone Code: High-Throughput HyperModified Peptide Analysis with Novel On-Line
LC-MS Coupled to Electron Transfer
Dissociation; Nicolas L. Young; Peter A.
DiMaggio; Mariana D. Plazas-Mayorca; Richard
C. Baliban; Christodoulos A. Floudas; Benjamin
A. Garcia; Princeton University, Princeton, NJ

ThOD pm 3:30 Sequencing of Bis-Arylhydrazone Cross-Linked Peptides by Electron Transfer Dissociation to Assess Protein-Protein Interactions; Myles Gardner¹²; Jennifer Brodbelt¹²; ¹The University of Texas, Austin, TX; ²The University of Texas, Austin, TX

ThOD pm 3:50 Electron Capture Dissociation de novo
Sequencing by C- and Z- Terminal Fragment
Discrimination Using Neutral-Radical
Reaction; Takashi Baba^{1,2}; Travis Greene¹; Gary
L. Glish¹; ¹University of North Carolina, Chapel
Hill, NC; ²Hitachi Ltd., Tokyo, Japan

ThOD pm 4:10 The Yeast Proteome Revealed by Electron
Transfer Dissociation and a Multiple ProteaseBased Shotgun Approach; Danielle L. Swaney;
Joshua J. Coon; University of Wisconsin,
Madison, WI

2:30-4:30, THURSDAY AFTERNOON CHARACTERIZING PTMs Exhibit Hall C

ThOE pm 2:30 Characterization of AMPylation on Threonine, Serine, and Tyrosine Using Tandem Mass Spectrometry; Yan Li; Rowaida Al-Eryani; Haydn L. Ball; UTSW, Dallas, TX

ThOE pm 2:50 Quantification of Histone Modifications upon Suz12 Deletion in Embryonic Stem Cells by High Mass Accuracy LTQ-CID/ETD-Orbitrap Mass Spectrometry; Hye Ryung Jung¹; Diego Pasini²; Marco Ruijken³; Linda Olsson²; Kristian Helin²; Ole N. Jensen¹; ¹University of Southern Denmark, Odense, Denmark; ²Biotech Research and Innovation Centre (BRIC), Copenhagen, Denmark; ³MsMetrix, Maarssen, The Netherlands

ThOE pm 3:10 Selected Reaction Monitoring (SRM) of Ubiquitin Isopeptide Linkages in Neurodegenerative Disease; Eric Dammer¹; Nicholas Seyfried¹; Ping Xu¹; Yair M. Gozal^{2,3}; Marla Gearing²; James J. Lah^{2,4}; Allan I. Levey^{2,4}; Junmin Peng^{1,2}; **IEmory University Department of Human Genetics, Atlanta, GA; **Center for Neurodegenerative Disease, Atlanta, GA; **Graduate Program in Neuroscience, Atlanta, GA; **Department of Neurology, Atlanta, GA

ThOE pm 3:30 Glycation Isotopic Labelling with 13C6Reducing Sugars for Quantitative Analysis of
Glycated Proteins; Feliciano Priego-capote¹;
Alexander Scherl¹; Yohann Couté²; Jean-charles
Sanchez³; ¹University of Geneva, Geneva,
Switzerland; ²Biomedical Proteomics Group,
Structural Biology an, Geneva, Switzerland;
³Geneva University, Geneva, Switzerland

ThOE pm 3:50 Characterization of Mycobacterium

Tuberculosis Membrane and Surface Exposed
Proteins by Liquid Chromatography Mass
Spectrometry-Based Proteomics Techniques;
Christina Bell 1,2; Mike Sweredoski 1; Sonja Hess 1;
Caltech, Pasadena, CA; Johannes Gutenberg-Universität, Mainz, Germany

ThOE pm 4:10 Revealing the Unexpected with Multi-Species Comparative Proteomics; Dumitru Brinza¹; Mary S. Lipton²; Kim K. Hixson²; Richard D. Smith²; Pavel Pevzner¹; Nuno Bandeira³; ¹University of California, San Diego, La Jolla, CA; ²PNNL / Battelle Northwest, Richland, WA; ³Center for Computational Mass Spectrometry, UCSD, La Jolla, CA

2:30-4:30, THURSDAY AFTERNOON MINIATURIZATION OF THE MASS SPECTROMETER Room 103

ThOF pm 2:30 Miniature Mass Spectrometers: Overview; R. Graham Cooks; Jason Harper; Nicholas Charipar; Guangming Huang; Liang Gao; Robert J. Noll; Zheng Ouyang; Purdue University, West Lafayette, IN

ThOF pm 2:50 Planar Electrode Ion Traps; <u>Daniel Austin;</u>
Zhiping Zhang; Ying Peng; Brett Hansen; Miao
Wang; Milton Lee; Aaron Hawkins; <u>Brigham</u>
Young University, Provo, UT

ThOF pm 3:10 Fundamentals of Miniature Quadrupole Mass Filters; Stephen Taylor¹; Boris Brkic¹; Adam Clare¹; Thomas J Hogan¹; Neil France²;

¹University of Liverpool, Liverpool, UK; ²Q-Technologies Ltd, Liverpool, UK

ThOF pm 3:30 In situ Mass Spectrometry for Marine
Applications: Present and Future; Tim Short¹;
Ryan J. Bell^{1,2}; Ashish Chaudhary^{1,2}; Friso H. W.
Van Amerom¹; Strawn K. Toler¹; ¹SRI
International, St Petersburg, FL; ²University of
South Florida, St Petersburg, FL

ThOF pm 3:50 Advances in Hand-Portable Gas
Chromatography-Toriodal Ion Trap Mass
Spectrometry; Milton L. Lee; Brigham Young
University, Provo, UT

ThOF pm 4:10

Development, Characterization and
Optimization of a Multiple Source Rectilinear
Ion Trap Miniature Mass Spectrometers; Liang
Gao; Jason Harper; Guangming Huang; Sameer
Kothari; Nathan Sanders; R. Graham cooks;
Zheng Ouyang; Purdue University, West
Lafayette, IN

2:30-4:30, THURSDAY AFTERNOON MS AND NANO-SCIENCE/NANO-TECHNOLOGY Room 113

ThOG pm 2:30 Nanostructure-Initiator Mass Spectrometry
(NIMS) Imaging: Direct Analysis of
Endogenous and Exogenous Metabolites in
Tissues; Hin-koon Woo; Oscar Yanes; Gary J
Patti; Wilasinee Uritboonthai; Junefredo Apon;
Gary Siuzdak; The Scripps Research Institute, La
Jolla, CA

ThOG pm 2:50 Field Enhanced Optimization of MALDI-TOF-MS Sample Preparation for Peptides Analysis
Using Induction Based Fluidics (IBF); Julie
Harmon; Paul Tate; Kevin J Clifford; Ted
Gauthier; University of South Florida, Tampa, FL

ThOG pm 3:10 Microfluidic-Based NanoLC/QQQ for High-Sensitivity Quantification of Pharmaceutical Molecules in Small Volumes of Whole Blood; Stephan Buckenmaier; Lukas Trojer; Agilent Technologies, Waldbronn, Germany

ThOG pm 3:30 Characterization of Free-Standing Nano-Objects Using Single Impact Cluster-SIMS;

Veronica Pinnick¹; Stanislav Verkhoturov¹;

Leonid Kaledin²; Emile A. Schweikert¹; ¹Texas

A&M University, College Station, TX; ²Argonide

Corporation, Sanford, FL

ThOG pm 3:50 Quantitative Proteomic Analysis of Mouse
Lymph Nodes Exposed to Titanium Dioxide
Nanoparticles; Yuan Gao; Neera V. Gopee;
Ricky D. Holland; Paul C. Howard; Li-Rong Yu;
National Center for Toxicological Research/FDA,
Jefferson, AR

ThOG pm 4:10 Multiplexed Tracking of Functionalized Gold
Nanoparticles in Biological Systems Using
Laser Desorption/Ionization Mass
Spectrometry (LDI-MS); Zhengjiang Zhu; Oscar
R. Miranda; Vincent M. Rotello; Richard Vachet;
University of Massachusetts Amherst, Amherst,

4:45 –5:30 PM, MONDAY PLENARY LECTURE Exhibit Hall C

Fostering Creativity



Richard N. Zare, Stanford University